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New free energy and susceptibility inequalities for the Ising-, XY- and Heisenberg-models and the problem of phase transition

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Abstract. For the d-dimensional spin $\frac{1}{2}$ Ising free energy and susceptibility upper and lower bounds have been constructed in the case of ferromagnetic and antiferromagnetic, nearest neighbour coupling. In the antiferromagnetic case the bounds belonging to the free energy or partition function are generated with help of the related chemical potential $\ln (Z_\Lambda/Z_{\Lambda-1})$. These bounds prove the existence of the free energy of antiferromagnetic type in the thermodynamic limit. If the coupling is the ferromagnetic type, then the d-dimensional free energy or susceptibility is bounded from above or from below by lower dimensional ones. For dimensionality $d > 2$ the bounds are also 2-dimensional, which prove the existence of finite magnetization (broken phase) below the transition temperature and that by Szegö–Kac theorem. These results have been applied to the d-dimensional, quantum Heisenberg- and XY-models and to the d-dimensional XY-model with homogeneous or inhomogeneous magnetic field in the z-direction. Assuming ferromagnetic coupling, the existence of finite magnetization is proved in these $d \geq 2$-dimensional quantum models.

1. Introduction

The partition function Z_Λ of the Ising model can be handled also by the standard cluster integral treatment of the imperfect gas. To obtain an alternating series of upper and lower bounds for the free energy of the Ising model with antiferro coupling one must make purely mathematical considerations for the expansion of Z_Λ. The mathematical tool [1] to the constructions of the bounds is given by the application of Lieb's inequalities [2] to the Ising model. The interest in the bounds lies in the fact that they allow to make strict conditions for continuous phase transition in the quantum mechanical XY-model with inhomogeneous magnetic field in the z-direction [3].

The mathematical preliminaries to the program can be formulated in a lemma:

Let f_k be a set of real functions, $k = 1, 2, \ldots, N$ such that $0 > f_k > -1$ for all k. If we define the function

$$I(s) = \prod_{k=1}^{N} (1 + sf_k) = \sum_{n=0}^{N} s^n A_n(\{f_n\}) \tag{1.1}$$

with

$$A_n(\{f_n\}) = \sum_{\{k_1, \ldots, k_n\}} f_{k_1} \cdots f_{k_n}, \quad A_0 = 1 \tag{1.2}$$

where we sum over all distinct n-tuples $k_1, \ldots, k_n$.

One has

Lemma 1.1. *If* $0 < s < 1$ *then holds*

$$I(s) \lesseqgtr \sum_{n=0}^{M} s^n A_n(\{f_k\}) \tag{1.3}$$

where $0 < M < N$ *and the* $>$ *sign is valid for odd* M *and* $<$ *sign for even* M.

The proof of this Lemma is given in references [1, 2] and will not be considered here, but we will apply directly the theorem to the problems studied in the next section.

If the $f_k - s$ in equation (1.1) are all positive semidefinite then all the inequalities in (1.3) become lower bounds. This situation is also of interest for the Ising model with ferromagnetic coupling. In this case one can derive lower bounds for the partition function and susceptibility. The lower bound to the d-dimensional partition function is given by lower dimensional ones, which is the case also for the susceptibility. Similar considerations have been made by Guerra, Rosen and Simon [4], see also reference [5]. In this latter case, upper bounds to the partition function and to the susceptibilities can be constructed with help of the Cauchy–Schwarz inequalities. These bounds are given also by lower dimensional systems.

Let us introduce here the d-dimensional, infinite lattice by Z^d and a bounded region in Z^d by Λ_{d_1}, $d_1 \leq d$. Further, the configuration energy H_{Λ_d} of the Ising model with constant, nearest neighbour coupling is defined as

$$H_{\Lambda_d} = \tfrac{1}{2} \sum_{\{k,l\} C \Lambda_d} v_{kl}[2n_k - 1_k][2n_l - 1_l], \tag{1.4a}$$

and

$$v_{kl} = \begin{Bmatrix} v > 0 & \text{n.n.} & \text{antiferro-coupling} \\ v < 0 & \text{n.n.} & \text{ferro-coupling} \end{Bmatrix} \text{ on } Z^d \tag{1.4b}$$

in the region $\Lambda_d \cdot n_k$ takes the values $\{0, 1\}$ for all $k \in \Lambda_d$. The lattice spin σ_k on site k is defined by

$$\sigma_k = 2n_k - 1_k. \tag{1.5}$$

The configurational energy equation (1.4) has a term which is bilinear in n_k and is the interesting one for our considerations in the next sections. In the equations (1.4 and 1.5) the indices k and l denote d-dimensional vectors: $k = \{k_1, k_2, \ldots, k_d\}$. The unit cell of Z^d is a hypercube; along the edges of the unit cell the interaction strengths are equal. We assume periodic boundary condition on Λ_d, which are essential in the third and fourth section.

2. Upper and lower bounds for the partition function with $v > 0$

In the bounded region Λ_d we define the partition function of H_{Λ_d} equation (1.4) by

$$Z_{\Lambda_d} = 2^{-\Lambda_d} \operatorname{Tr} \{\exp(-\beta H^0_{\Lambda_d}) I_{\Lambda_d}(n_1, \ldots, n_{\Lambda_d})\} \tag{2.1}$$

where

$$H^0_{\Lambda_d} = \tfrac{1}{2} \sum_{\{k,l\}\in\Lambda(d)} v_{kl}[1_k - 4n_k], \quad (v_{kl} > 0), \tag{2.2}$$

$$I_{\Lambda_d}(n_1, \ldots, n_{\Lambda_d}) = \prod_{\{k,l\}\in\Lambda(d)} [1 + f_{kl}]. \tag{2.3}$$

The f_{kl} are the Mayer functions belonging to the model equation (1.4):

$$f_{kl} = \exp[-4\beta v_{kl} n_k n_l] - 1. \tag{2.4}$$

In view of the definition equation (2.1), the free energies F_{Λ_d} and F_{Λ_d-1} fulfil the relation

$$\frac{Z_{\Lambda_d}}{Z_{\Lambda_d-1}} = \exp[-\beta(F_{\Lambda_d} - F_{\Lambda_d-1})] \tag{2.5}$$

for large Λ. In the circular bracket of the above equation (2.5), the difference $F_{\Lambda_d} - F_{\Lambda_d-1}$ corresponds a chemical potential of the system in view of

$$\frac{\partial F_{\Lambda_d}}{\partial \Lambda_d} = \lim_{\Delta\to 0} \frac{F_{\Lambda_d} - F_{\Lambda_d-\Delta}}{\Delta}. \tag{2.6}$$

Because Λ_d is large, Δ corresponds to the one of F_{Λ_d-1}. On the other hand, one has

$$F_{\Lambda_d} = \sum_{x=1}^{\Lambda_d} [F_x - F_{x-1}]; \qquad x, \Lambda_d \subset Z^d. \tag{2.7}$$

Our aim is to construct upper and lower bounds to the free energy per site

$$f = \lim_{\Lambda_d\to\infty} \frac{1}{\Lambda_d} F_{\Lambda_d}$$

by virtue of equations (2.5–2.7). Let us at first collect some results concerning the partition function and free energy:

Theorem 2.1. *If the coupling constant of $H_{\Lambda_d} v_{kl} > 0$ equation (1.4), then H_{Λ_d} – related partition function Z_{Λ_d} has the alternating bound properties*

$$Z_{\Lambda_d} < Z_{\Lambda_d-1} \tag{2.8a}$$

$$Z_{\Lambda_d} > Ch(\beta z v) Z_{\Lambda_d-1} - \frac{z}{2}\exp[\beta(\tfrac{3}{2}z - 2)v] Sh(2\beta v) Z_{\Lambda_d-2} \tag{2.8b}$$

$$Z_{\Lambda_d} < Ch(\beta z v) Z_{\Lambda_d-1} - \frac{z}{2}\exp[\beta(\tfrac{3}{2}z - 2)v] Sh(2\beta v) Z_{\Lambda_d-2} + \frac{z^2}{2}\exp[\beta(\tfrac{9}{2}z - 4)v] Sh^2(2\beta v) Z_{\Lambda_d-3} \tag{2.8c}$$

⋮

etc.

(z: number of nearest neighbours); further the free energy per site $f = \lim_{\Lambda_d\to\infty} 1/\Lambda_d\, F_{\Lambda_d}$ satisfies

$$\ln\left[\frac{b}{2a} + \sqrt{\frac{b^2}{4a^2} - \frac{1}{a}}\right] < \beta f < \ln\left[\frac{b}{2a} - \sqrt{\frac{b^2}{4a^2} - \frac{1}{a}}\right] \tag{2.9}$$

for certain parameter values βv, $\beta = [k_B T]^{-1}$. *a and b are:*

$$a = \frac{z}{2} \exp\left[\beta\left(\tfrac{3}{2} z - 2\right)v\right] Sh(2\beta v) \quad \text{and} \quad b = Ch(\beta z v).$$

The alternating bound property inequalities (2.8) can be established as follows: From the definition equation (2.3) one has

$$I_{\Lambda_d}(n_1, \ldots, n_{\Lambda_d}) = \prod_{j=2}^{\Lambda_d} (1 + f_{1j}) I_{\Lambda_d - 1}(n_2, \ldots, n_{\Lambda_d}). \tag{2.10}$$

Since $I_{\Lambda_d - \Delta} > 0$ for $\Delta = 0, 1, 2, \ldots, \Lambda_d - 1$ and f_{ij} satisfies the inequality

$$0 > f_{ij} > -1, \tag{2.11}$$

then it follows by lemma 1.1

$$I_{\Lambda_d} < I_{\Lambda_d - 1} \tag{2.12a}$$

$$I_{\Lambda_d} > \left(1 + \sum_{j=2}^{\Lambda_d} f_{1j}\right) I_{\Lambda_d - 1} \tag{2.12b}$$

$$I_{\Lambda_d} < \left(1 + \sum_{j=2}^{\Lambda_d} f_{1j} + \sum_{\{kl\}}^{\Lambda_d} f_{1k} f_{1l}\right) I_{\Lambda_d - 1} \tag{2.12c}$$

$$\vdots$$

etc.

Multiplying equation (2.12a) with $2^{-\Lambda_d} \exp(-\beta H^{\circ}_{\Lambda_d})$ and taking the trace over the gained expression, one gets the inequality (2.8a). Similarly one gets

$$Z_{\Lambda_d} > 2^{-\Lambda_d} \operatorname{Tr}\{\exp(-\beta H^{\circ}_{\Lambda_d}) I_{\Lambda_d - 1}\} + 2^{-\Lambda_d} \operatorname{Tr}\{\exp(-\beta H^{\circ}_{\Lambda}) z f_{12} I_{\Lambda_d - 2}\} \tag{2.13}$$

by inserting

$$f_{12} I_{\Lambda_d - 1} > f_{12} I_{\Lambda_d - 2} \tag{2.14}$$

into inequality (2.12b). Inequality (2.14) follows by inequalities (2.11–2.12a). The inequality (2.13) immediately results from (2.8b). On the right hand side of inequality (2.8c) the first two terms are derived along inequalities (2.12b–2.14), as we have done for the inequality (2.8b). The last term of inequality (2.8c) is gained by the inequality

$$\begin{aligned} &2^{-\Lambda_d} \operatorname{Tr}\left\{\exp(-\beta H^{\circ}_{\Lambda_d}) \sum_{\{kl\}} f_{1k} f_{1l} I_{\Lambda_d - 1}\right\} \\ &\quad = 2^{-\Lambda_d} \operatorname{Tr}\{\exp(-\beta H^{\circ}_{\Lambda_d}) z(z-1) f_{12} f_{13} I_{\Lambda_d - 1}\} \\ &\quad < 2^{-\Lambda_d} \operatorname{Tr}\{\exp(-\beta H^{\circ}_{\Lambda_d}) z(z-1) f_{12} f_{13} I_{\Lambda_d - 3}\} \end{aligned} \tag{2.15}$$

and the evaluation of the right hand side of equation (2.15) proves the inequality (2.8c).

The second part of the Theorem 2.1, inequality (2.9) follows from the inequalities (2.8b–2.8c). It holds

$$1 > b\frac{Z_{\Lambda_d-1}}{Z_{\Lambda_d}} - a\frac{Z_{\Lambda_d-2}}{Z_{\Lambda_d}} = b\exp\left[\beta\frac{\partial F_{\Lambda_d}}{\partial_{\Lambda_d}}\right] - a\exp\left[2\beta\frac{\partial F_{\Lambda_d}}{\partial_{\Lambda_d}}\right] \tag{2.16a}$$

$$1 < b\exp\left[\beta\frac{\partial F_{\Lambda_d}}{\partial_{\Lambda_d}}\right] - a\exp\left[2\beta\frac{\partial F_{\Lambda_d}}{\partial_{\Lambda_d}}\right] + 2a^2\exp\left[\frac{3}{2}\beta z v\right]\exp\left[3\beta\frac{\partial F_{\Lambda_d}}{\partial_{\Lambda_d}}\right] \tag{2.16b}$$

by applying equations (2.5–2.6). The above inequality of second degree is solved easily for the unknown variable

$$\exp\left[\beta\frac{\partial F_{\Lambda_d}}{\partial_{\Lambda_d}}\right].$$

One gets

$$\ln\left[\frac{b}{2a} + \sqrt{\frac{b^2}{4a^2} - \frac{1}{a}}\right] < \beta\frac{\partial F_{\Lambda_d}}{\partial_{\Lambda_d}} < \ln\left[\frac{b}{2a} - \sqrt{\frac{b^2}{4a^2} - \frac{1}{a}}\right]. \tag{2.17}$$

From here the inequality (2.9) follows by integration over Λ_d.

3. Bounds on the ferromagnetic partition function and susceptibility

The basis of Theorem 2.1 are the inequalities (2.12), which are a consequence of the Lemma 1.1. As it has been pointed out in section 1, the upper bounds of Lemma 1.1 change to lower ones, because $f_n > 0$ for $v_{kl} < 0$.

This has the consequence that the inequalities equation (2.12) become lower bounds,

$$I_{\Lambda_d}(n_1,\ldots,n_{\Lambda_d}) > I_{\Lambda_d-1}(n_2,\ldots,n_{\Lambda_d})$$

$$I_{\Lambda_d}(n_1,\ldots,n_{\Lambda_d}) > \left(1 + \sum_j f_{1j}\right) I_{\Lambda_d-1}(n_2,\ldots,n_{\Lambda_d}) \tag{3.1}$$

$$I_{\Lambda_d}(n_1,\ldots,n_{\Lambda_d}) > \left(1 + \sum_j f_{1j} + \sum_{kl} f_{1k}f_{1l}\right) I_{\Lambda_d-1}(n_2,\ldots,n_{\Lambda_d})$$

$$\vdots$$

etc.

in the ferromagnetic case, which is on the other hand a consequence of equation (2.10) and of the inequality

$$f_{kl} = \exp\left[-4\beta v_{kl} n_k n_l\right] - 1 > 0 \quad (v_{kl} < 0). \tag{3.2}$$

From the above inequalities (3.1–3.2) it is clear that the partition function Z_{Λ_d} is bounded from below by Z_{Λ_d-n}, $\Lambda_d > n > 1$. So far the dimensionality of the system has not been considered explicitly; we will take this into account now. The model (1.4) with $v_{kl} < 0$ is defined in the bounded region $\Lambda_d \subset Z^d$. The hypercube Λ_d has a hypersurface Λ_{d-1}.

For the subspaces Λ_{d_1} and Λ_{d_1} with $d = d_1 + d_2$ the inequality (3.1) can be generalized so that it has the consequences:

Theorem 3.1. *Let Λ_{d_1} and Λ_{d_2} with $d_1 = d - 1$ and $d_2 = 1$ two bounded subsets of Z^d, so that $\Lambda_1\Lambda_{d-1} = \Lambda_d \subset Z^d$. Then it holds*

$$I_{\Lambda_d} > \prod_{j=1}^{N_d} I_{\Lambda_{d-1}}(j) \tag{3.3}$$

where N_d is a lattice point in the dth one dimensional subspace with the cyclic boundary condition $N_d + 1 = 1$. Further, the partition function Z_{Λ_d} fulfils the inequalities

$$Z_{\Lambda_d} > (Z_{\Lambda_{d-1}})^{\Lambda_1(d)} > (Z_{\Lambda_{d-2}})^{\Lambda_1(d)\Lambda_1(d-1)} \dots > (Z_{\Lambda_1})^{\prod_{j=2}^{d}\Lambda_1(j)}; \tag{3.4}$$

and the d-dimensional susceptibility belonging to Z_{Λ_d} is bounded from below by a sequence of lower dimensional susceptibilities, which belong to $Z_{\Lambda_{d-1}}, \dots$ and Z_{Λ_1}:

$$d\hat{\chi}_d(q_1 \mid v) > (d-1)\hat{\chi}_{d-1}(q_1 \mid v) > (d-2)\hat{\chi}_{d-2}(q_1 \mid v) > \cdots > \chi_1(q_1 \mid v). \tag{3.5}$$

$\hat{\chi}_d(q_1 \mid v)$ is the 1-dimensional Fourier-transform of

$$\beta\langle\sigma_k\sigma_l\rangle_d = \beta\langle\sigma_{(k_1k_2\dots k_d)}\sigma_{(l_1k_2\dots k_d)}\rangle_d:$$

$$\hat{\chi}_d(q_1 \mid v) = \frac{1}{\Lambda_1}\sum_{k_1}\exp\,[iq_1(R_{k_1} - R_{l_1})]\beta\langle\sigma_{(k_1k_2\dots k_d)}\sigma_{(l_1k_2\dots k_d)}\rangle_d \tag{3.6}$$

where k and l are d-dimensional vectors as indicated, $\langle\cdots\rangle_d$ a d-dimensional average and $\beta = [k_BT]^{-1}$.

Special cases: Assuming $\Lambda^{1(j)} \equiv \Lambda_1$ for all $j = 1, \dots, d$ then the 3- and 4-dimensional partition functions fulfil the inequalities

$$Z_{\Lambda_3} > (Z_{\Lambda_2})^{\Lambda_1} > (Z_{\Lambda_1})^{\Lambda_1^2}, \tag{3.7}$$

$$Z_{\Lambda_4} > (Z_{\Lambda_3})^{\Lambda_1} > (Z_{\Lambda_2})^{\Lambda_1^2} > (Z_{\Lambda_1})^{\Lambda_1^3} \tag{3.8}$$

and the associated susceptibilities obey the relations

$$3\hat{\chi}_3(q_1 \mid v) > 2\hat{\chi}_2(q_1 \mid v) > \hat{\chi}_1(q_1 \mid v), \tag{3.9}$$

$$4\hat{\chi}_4(q_1 \mid v) > 3\hat{\chi}_3(q_1 \mid v) > 2\hat{\chi}_2(q_1 \mid v) > \hat{\chi}_1(q_1 \mid v). \tag{3.10}$$

Proof: The assertion equation (3.3) can be established by splitting up the model configuration energy equation (1.4) into two contributions:

$$H_{\Lambda_d} = H_{\Lambda^{d-1}} + H_{\Lambda^1} \tag{3.11}$$

where $H_{\Lambda^{d-1}}$ and H_{Λ^1} are:

$$H_{\Lambda^{d-1}} = \tfrac{1}{2}\sum_{k',l'} v_{k'l'}[2n_{k'} - 1_{k'}][2n_{l'} - 1_{l'}], \tag{3.12a}$$

$$H_{\Lambda^1} = \tfrac{1}{2}\sum_{k'',l''} v_{k''l''}[2n_{k''} - 1_{k''}][2n_{l''} - 1_{l''}] \tag{3.12b}$$

with $k' = \{k_1, \ldots, k_{d-1}, k_d = l_d\}$, $l' = \{l_1, \ldots, l_{d-1}, l_d = k_d\}$, $k'' = \{k_1 = l_1, \ldots, k_{d-1} = l_{d-1}, k_d\}$ and $l'' = \{l_1 = k_1, \ldots, l_{d-1} = k_{d-1}, l_d\}$. The above equations (3.12) contain constant nearest neighbour coupling.

Now we can define I_{Λ^1}, belonging to H_{Λ^1}, by the expression:

$$I_{\Lambda^1} = \prod_{\{k''l''\}} (1 + f_{k''l''}) > 1. \tag{3.13}$$

From equations (3.11–3.12) it follows that I_{Λ_d} can be expressed as a product from I_{Λ^1} and $I_{\Lambda^{d-1}}$:

$$I_{\Lambda_d} = I_{\Lambda^1} \cdot I_{\Lambda^{d-1}}, \tag{3.14}$$

where $I_{\Lambda^{d-1}}$ is defined similarly as I_{Λ^1} equation (3.13) by $H_{\Lambda^{d-1}}$. The definition equation (3.12) and the fact $f_{k''l''} \geq 0$ tells us:

$$I_{\Lambda_d} > I_{\Lambda_{d-1}}. \tag{3.15}$$

Note that H_{Λ^1} and $H_{\Lambda^{d-1}}$ do depend on the volume Λ_d as H_{Λ_d} does. Therefore, this is also the case for I_{Λ^1} and $I_{\Lambda^{d-1}}$. It follows directly from the above equations that the inequality

$$\mathrm{Tr}\,\{\exp(-\beta H_{\Lambda_d})\} > \mathrm{Tr}\,\{\exp(-\beta H_{\Lambda_{d-1}})\} \tag{3.16}$$

is satisfied. Now $H_{\Lambda^{d-1}}$ resp. H_{Λ^1} contain 1- resp. $(d-1)$-dimensional dummy summation. Therefore, the first inequality of (3.4) follows: $Z_{\Lambda_d} > (Z_{\Lambda_{d-1}})^{\Lambda^{1(d)}}$, and the sequence of the inequalities (3.4) follows by recurrence relation.

The sequence of inequalities (3.4) is also equivalent to

$$\frac{1}{\Lambda_d} \ln Z_{\Lambda_d} > \frac{1}{\Lambda_{d-1}} \ln Z_{\Lambda_{d-1}} > \frac{1}{\Lambda_{d-2}} \ln Z_{\Lambda_{d-2}} > \cdots > \frac{1}{\Lambda_1} \ln Z_{\Lambda_1}, \tag{3.17}$$

where we used $\Lambda_d = \prod_{j=1}^{d} \Lambda^{1(j)}$

Using the identity

$$\begin{aligned} \frac{1}{\Lambda_d} \ln Z_{\Lambda_d} &= \frac{1}{\Lambda_d} \sum_{k,l} \int_0^1 d\lambda v_{kl} \langle \sigma_k \sigma_l \rangle_d(\lambda v) \\ &= \frac{1}{\Lambda_d} \sum_{k,l} \int_0^1 d\lambda v_{kl}\, \mathrm{Tr}_{\Lambda_d}\{\rho_{\Lambda_d}(\lambda v) \sigma_k \sigma_l\} \end{aligned} \tag{3.18}$$

and the translation invariance of the system one obtains the sequence of susceptibility inequalities (3.5) by the facts:

$$\hat{\sigma}_{q_1} \hat{\sigma}_{-q_1} \geq 0, \tag{3.19a}$$

$$\exp\{-\beta H_{\Lambda_d}\} > \exp\{-\beta H_{\Lambda_{d-1}}\} > \cdots > \exp\{-\beta H_{\Lambda_1}\}. \tag{3.19b}$$

The equations (3.15–3.19) prove Theorem 3.1.

Let us show that the d-dimensional partition function Z_{Λ_d} and its related susceptibility can be bounded from above by lower dimensional ones.

One has:

Theorem 3.2. *Let $H_{\Lambda_d} = H_{\Lambda_{d-1}} + H_{\Lambda_1}$ in the sense of equations (3.11–3.12). Then:*

$$\frac{1}{\Lambda_d} \ln Z_{\Lambda_d}(v) \leq \frac{1}{2\Lambda_{d-1}} \ln Z_{\Lambda_{d-1}}(2v) + \frac{1}{2\Lambda_1} \ln Z_{\Lambda_1}(2v) \tag{3.20}$$

and the susceptibilities $\hat{\chi}_d(q_1 \mid v)$, $\hat{\chi}_{d-1}(q_1 \mid 2v)$ and $\hat{\chi}_1(q_1 \mid 2v)$ satisfy the inequality

$$d \cdot \hat{\chi}_d(q_1 \mid v) \leq (d-1)\hat{\chi}_{d-1}(q_1 \mid 2v) + \hat{\chi}_1(q_1 \mid 2v). \tag{3.21}$$

Proof: By Cauchy–Schwarz inequality one has

$$Z_{\Lambda_d}(v) \leq [Z_{\Lambda_{d-1}}(2v)]^{1/2 \cdot \Lambda_1} \cdot [Z_{\Lambda_1}(2v)]^{1/2 \cdot \Lambda_{d-1}} \tag{3.22}$$

and (3.21) follows immediately, because Z_{Λ_x} is defined with an x-dimensional configuration energy. The equations (3.6) and (3.18–3.19) with the positive definity of $\hat{v}_{q_x}$ (q_x: x-dimensional wave vector) leads to the inequality (3.21), where we used again translation invariance.

The two above stated Theorems 3.1 and 3.2 have consequences: Let us denote

$$-\beta f_d(v) = \lim_{\Lambda_d \to \infty} \frac{1}{\Lambda_d} \ln Z_{\Lambda_d}(v) \tag{3.23}$$

the thermodynamic limit of the free energy per site and Z_{Λ_d} is defined with the configuration energy equation (1.4). Then:

Corollary 3.3. *The d-dimensional free energy per site f_d equation (3.23) of the ferromagnetic Ising model with constant nearest neighbour coupling fulfils the sequence of inequalities:*

$$-\tfrac{1}{2}\beta f_{d-1}(2v) - \tfrac{1}{2}\beta f_1(2v) > -\beta f_d(v) > -\beta f_{d-1}(v) > \cdots > -\beta f_1(v), \tag{3.24}$$

and therefore the free energy per site $f_d(v)$ is finite and the inequalities (3.5) and (3.21) remain in the thermodynamic limit.

This corollary follows from the Ising and Onsager solutions of the 1- and 2-dimensional Ising models.

4. Applications

Finally, in this section we consider some further consequences of our results. Let us consider the properties of positive definite functions at first.

A function $f(x)$ is called positive definite if it is continuous on $\mathbb{R}^d$ and has the property

$$\sum_{\mu, \nu \in Z^d} \rho_\mu f(x_\mu - x_\nu)\overline{\rho^\nu} \geq 0 \quad (Z^d \in \mathbb{R}^d) \tag{4.1}$$

for any points $x_\mu \in \mathbb{R}^d$, and any numbers $\rho_\mu \in \mathbb{C}^d$. Each function $f(x)$ with the above properties is positive definite. This fact is related to Fourier–Stiltjes integrals, e.g. each characteristic function

$$f(x) = \int \exp(ixq)\, dV(q) \tag{4.2}$$

is positive definite. There holds

Theorem 4.1. [6]: *Let $\hat{p}(q)$ be periodic, positive definite and integrable (over the d-dimensional Brillouin-zone). In order that $f(x)$ can be represented over $\mathbb{R}^d$ by the expression*

$$f(x) = \int e^{ixq}\hat{p}(q)\, dq \quad (Z^d \subset \mathbb{R}^d) \tag{4.3}$$

it is necessary and sufficient for $f(x)$ to be positive definite.

It is the direct consequence of the above theorem that the inequalities equations (3.5) and (3.21) remain valid in direct space also. One has:

Corollary 4.2. *In any d-dimensional spin $\frac{1}{2}$ Ising ferromagnet with constant nearest neighbour interaction*

$$\begin{aligned} &(d-1)\langle\sigma_{(k_1\ldots k_{d-2}k_{d-1})}\sigma_{(k_1\ldots k_{d-1}l_{d-1})}\rangle_{d-1}(2v) + \langle\sigma_{k_1}\sigma_{l_1}\rangle_1(2v) \\ &\geq d\langle\sigma_{(k_1\ldots k_{d-1}k_d)}\sigma_{(k_1\ldots k_{d-1}l_d)}\rangle_d(v) \\ &> (d-1)\,\langle\sigma_{(k_1\ldots k_{d-2}k_{d-1})}\sigma_{(k_1\ldots k_{d-2}l_{d-1})}\rangle_{d-1}(v) > \cdots > \langle\sigma_{k_1}\sigma_{l_1}\rangle_1(v) \geq 0. \end{aligned} \tag{4.4}$$

Therefore, the d-dimensional spin $\frac{1}{2}$ Ising correlation function of ferromagnetic type is positive on a one-dimensional line and is bounded from below by a sequence of lower dimensional, positive definite correlation functions. The positive definity of the correlation function is a special case of Griffith's first inequality [7]. *Further, the lower dimensional upper bound of the d-dimensional Ising correlation function of ferromagnetic type proves the existence of the higher dimensional system.*

The 2-dimensional lower bound to the d-dimensional correlation function proves the existence of finite magnetization in the d-dimensional spin $\frac{1}{2}$ Ising system of ferromagnetic type by the Szegö–Kac theorem [8]:

$$\lim_{k_d - l_d \to \infty} \langle\sigma_{k''}\sigma_{l''}\rangle_d(v) > \frac{2}{d} \lim_{k_2 - l_2 \to \infty} \langle\sigma_{k_1k_2}\sigma_{k_1l_2}\rangle_2(v) > 0$$

for appropriate choice of the nearest neighbour coupling constant v. The Szegö–Kac theorem is discussed in the Appendix.

We are now ready to apply the above Theorem 4.1 and the Corollary 4.2 to the d-dimensional quantum XY- and Heisenberg models. For the free energy and susceptibility of these models singular upper and lower bounds have been given in d-dimension [9]. The bounds were given by the d-dimensional spin $\frac{1}{2}$ Ising model free energy and susceptibility of ferromagnetic type. Let us define the Fourier transform of the correlation functions by

$$\hat{\chi}_d^{\mathscr{H}}(q_1 \mid \lambda v) = \mathrm{Tr}\,\{\rho_{\mathscr{H}}(\lambda v)\hat{\sigma}^{\alpha}_{q_1}\hat{\sigma}^{\alpha}_{-q_1}\}, \quad \alpha = x, y, z \tag{4.5}$$

for the d-dimensional Heisenberg model and by

$$\hat{\chi}_d^{xy}(q_1 \mid \lambda v) = \mathrm{Tr}\,\{\rho^{xy}(\lambda v)\hat{\sigma}^{\beta}_{q_1}\hat{\sigma}^{\beta}_{-q_1}\}, \quad \beta = x, y \tag{4.6}$$

for the d-dimensional XY-model. The Fourier-transform of the Pauli-spin operators σ_k^{α} is defined in a similar way as in equation (3.6). $\rho_{\mathscr{H}}(\lambda v)$ and $\rho^{xy}(\lambda v)$ are the density operators belonging to the isotropic Heisenberg and XY-models. The Hamiltonians are defined with constant nearest neighbour coupling of ferromagnetic type. Then:

Theorem 4.3. *The d-dimensional Heisenberg and XY-correlation functions equations (4.5–4.6) satisfy the inequalities* [9]:

$$6\hat{\chi}_d(q_1 \mid 2v) \geq \hat{\chi}_d^{\mathscr{H}}(q_1 \mid v) \geq \hat{\chi}_d(q_1 \mid \tfrac{1}{2}v), \tag{4.7}$$

$$2\hat{\chi}_d(q_1 \mid 2v) \geq \tfrac{1}{2}\hat{\chi}_d^{xy}(q_1 \mid v) \geq \tfrac{1}{2}\hat{\chi}_d(q_1 \mid \tfrac{1}{2}v). \tag{4.8}$$

Thus, one has the following application of the Theorems 4.1 and 4.3 and Corollary 4.2:

Corollary 4.4. *In any d-dimensional XY- and Heisenberg ferromagnet with constant nearest neighbour interaction*

$$\begin{aligned} 6\langle\sigma_{k''}^x\sigma_{l''}^x\rangle_d(2v) &\geq \langle\sigma_{k''}^x\sigma_{l''}^x\rangle_{d,\mathscr{H}}(v) \geq \langle\sigma_{k''}^x\sigma_{l''}^x\rangle_d(\tfrac{1}{2}v) \\ &> \frac{2}{d}\langle\sigma_{k''}^x\sigma_{l''}^x\rangle_2(\tfrac{1}{2}v) \geq 0, \end{aligned} \tag{4.9}$$

$$\begin{aligned} 2\langle\sigma_{k''}^x\sigma_{l''}^x\rangle_d(2v) &\geq \tfrac{1}{2}\langle\sigma_{k''}^x\sigma_{l''}^x\rangle_{d,xy}(v) \geq \tfrac{1}{2}\langle\sigma_{k''}^x\sigma_{l''}^x\rangle_d(\tfrac{1}{2}v) \\ &> \frac{1}{d}\langle\sigma_{k''}^x\sigma_{l''}^x\rangle_2(\tfrac{1}{2}v) \geq 0. \end{aligned} \tag{4.10}$$

We have defined $\langle\sigma_{k''}^x\sigma_{l''}^x\rangle_{d,\mathscr{H}}(v)$ and $\langle\sigma_{k''}^x\sigma_{l''}^x\rangle_{d,xy}$ as the one dimensional Fourier transform of $\hat{\chi}_d^{\mathscr{H}}(q_1 \mid v)$ and of $\hat{\chi}_d^{xy}(q_1 \mid v)$. Further, $k'' = \{k_1, k_2, \ldots, k_d\}$ and $l'' = \{l_1, k_2, \ldots, k_d\}$. It is clear by the Szegö–Kac theorem [8] again, that the magnetization in the $d \geq 2$-dimensional Heisenberg and XY-models is different from zero

$$\lim_{k_1 - l_1 \to \infty} \langle\sigma_{k''}^x\sigma_{l''}^x\rangle_{d,\mathscr{H}}(v) > \frac{2}{d} \lim_{k_1 - l_1 \to \infty} \langle\sigma_{k''}^x\sigma_{l''}^x\rangle_2(\tfrac{1}{2}v) > 0 \tag{4.11}$$

and

$$\lim_{k_1 - l_1 \to \infty} \langle\sigma_{k''}^x\sigma_{l''}^x\rangle_{d,xy} > \lim_{k_1 - l_1 \to \infty} \frac{2}{d}\langle\sigma_{k''}^x\sigma_{l''}^x\rangle_2(\tfrac{1}{2}v) > 0 \tag{4.12}$$

for appropriate coupling constant v. It follows:

Theorem 4.5. *The magnetization per site*

$$M_{d,\alpha} = \lim_{\Lambda_d \to \infty} \frac{1}{\Lambda_d} \langle \sum_{k} {}_{\Lambda_d} \sigma_k \rangle_{d,\alpha} \neq 0 \tag{4.13}$$

in the $d \geq 2$-dimensional Heisenberg ($\alpha \equiv \mathscr{H}$) and XY-model ($\alpha \equiv XY$) by an appropriate choice of coupling constant v.

The fact, that $M_{d,\alpha} \neq 0$ for $d \geq 2$, is a consequence of the relation $\lim_{k_1 - l_1 \to \infty} \langle\sigma_{k''}^x\sigma_{l''}^x\rangle_2(\tfrac{1}{2}v) = M^2 < M_{d,\alpha}^2$ below the critical temperature T_c, $M \sim A \mid (T_c - T)/T_c \mid^{1/8}$.

As in the Heisenberg and XY-models one has similar interest in the d-dimensional XY-model with homogeneous or inhomogeneous magnetic field in the z-direction, because of their relation to the *KDP*- and *BCS*-models. The existence of phase transition has been proven in these models [3]. We would like to discuss it in this context also. Let us define the correlation function of the d-dimensional XY-model with inhomogeneous magnetic field in the z-direction by

$$\langle \sigma^{\alpha}_{k''}\sigma^{\alpha}_{l''}\rangle_{d,\varepsilon}(\lambda v) = \mathrm{Tr}\,\{\rho^{\varepsilon}(\lambda v)\sigma^{\alpha}_{k''}\sigma^{\alpha}_{l''}\} \tag{4.14}$$

and the related Hamiltonian is

$$H^{\varepsilon}_{\Lambda_d} = -\tfrac{1}{2}\sum_{j\Lambda_d}(\sigma^z_j + \varepsilon_j)^2 + \tfrac{1}{2}\sum_{\substack{k.l\subset\Lambda_d\\ \alpha=x,y}} v_{kl}\sigma^{\alpha}_k\sigma^{\alpha}_l \tag{4.15}$$

with $v_{kl} \leq 0$. It is known that the one-dimensional Fourier transform $\hat{\chi}^{\varepsilon}_d(q_1 \mid v)$ of equation (4.14) fulfils the inequality

$$\hat{\chi}^{\varepsilon}_d(q_1 \mid v) \geq \hat{\chi}_d(q_1 \mid \tfrac{1}{4}v), \tag{4.16}$$

and if it holds that

$$-\lim_{\Lambda_d\to\infty}\left[\frac{1}{2\Lambda_d}\ln \mathrm{Tr}\left\{\exp\left(\frac{\beta}{2}H_{\Lambda_d}\right)\right\} + \frac{1}{\Lambda_d}\sum_{j\Lambda_d}\ln Ch(\beta\varepsilon_j)\right] \geq 0, \tag{4.17}$$

then:

Theorem 4.6. *If inequalities (4.16–4.17) are satisfied, then the correlation function equation (4.14) is bounded from below:*

$$\langle \sigma^{\alpha}_{k''}\sigma^{\alpha}_{l''}\rangle_{d,\varepsilon}(v) > \frac{2}{d}\langle \sigma^{x}_{k''}\sigma^{x}_{l''}\rangle_2(\tfrac{1}{4}v), \tag{4.18}$$

and the magnetization of the model equation (4.15) as a limit

$$0 < M^2 = \lim_{k_1-l_1\to\infty}\langle \sigma^{x}_{k''}\sigma^{x}_{l''}\rangle_2(\tfrac{1}{4}v) < \lim_{k_1-l_1\to\infty}\frac{d}{2}\langle \sigma^{\alpha}_{k''}\sigma^{\alpha}_{l''}\rangle_d(v) = \frac{d}{2}M^2_{d,\varepsilon} \tag{4.19}$$

exists below the transition temperature T_c.

Sketch of the proof: In reference [3] one has shown that the inequality (4.16) under the assumption of inequality (4.17) is fulfilled. Using inequality (4.16) in Theorem 4.1, and Corollary 4.2, the inequality (4.18) follows, from which equation (4.19) results. Therefore, it remains to show that the inequality (4.17) can be fulfilled; that this is the case follows from Theorem 2.1.

Similar thoughts can be applied also in lattice field and field theories.

Appendix

To prove the existence of the spontaneous magnetization of the 2-dimensional Ising model, one represents the correlation function as the Toeplitz determinant $D_{k_2-l_2}(f) = \langle \sigma_{k_1k_2}\sigma_{k_1l_2}\rangle_2(v)$ whose elements are the coefficients in the Laurent expression of a function $f(x)$.

Let $f(x)$ be positive, satisfying the Lipschitz condition and the derivative $f'(x)$ should exist. Then one has the Theorem:

Theorem [8]. *If $f(x)$ satisfies the above conditions, $G(f)$ denotes the geometric mean of $f(x)$ and $D_n(f)$ is the* n*th Toeplitz determinant associated with the function $f(x)$, then it holds*

$$\lim_{n\to\infty} \frac{D_n(f)}{[G(f)]^{n+1}} = \exp\left[\sum_{m=0}^{\infty} m\,|h_m|^2\right],$$

where

$$G(f) = \exp\left[\frac{1}{2\pi}\int_{-\pi}^{\pi} \ln f(x)\,dx\right]$$

and

$$\ln f(x) = \sum_{m=-\infty}^{+\infty} h_m \exp(imx).$$

In the case of the two-dimensional Ising model $G(f) = 1$ and

$$h_m = -h_{-m} = \frac{1}{2m}\left[-\left(\frac{Z_1}{Z_2^*}\right)^m - (Z_1 Z_2^*)^m + 2(-1)^m\right]$$

with $Z_1 = th(\beta J_1)$ and $Z_2 = th(\beta J_2)$ in the case of anisotropic coupling [10].

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