A New Class of Bounds for Correlation Functions in Euclidean Lattice Field Theory and Statistical Mechanics of Spin Systems

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Abstract

Starting from an extension of the Poisson bracket structure and Kubo-Martin-Schwinger-property of classical statistical mechanics of continuous systems to spin systems, defined on a lattice, we derive a series of, as we think, new and interesting bounds on correlation functions for general lattice systems. Our method is expected to yield also useful results in Euclidean Field Theory. Furthermore the approach is applicable in situations where other techniques fail, e.g. in the study of phase transitions without breaking of a **continuous** symmetry like $P(\phi)$-theories with $\phi(x)$ scalar.

1. Introduction

In more recent times it has become more and more apparent that the natural Poisson bracket structure of systems of classical point particles is of considerable conceptual **and** practical value in the investigation of all sorts of questions being related to e.g. phase transitions in thermal equilibrium systems, transport equations and the like (see e.g. refs. [1] to [8]).

One reason of its usefulness derives from the fact that both the classical equilibrium condition (more specifically, the so-called Kubo-Martin-Schwinger (KMS)-condition; cf. e.g. [9]) **and** the concept of symmetry (breaking) can be very neatly implemented by this structure.

The KMS-condition in the regime of classical statistical mechanics of point particles reads:

$$< \{A, B\} >= \beta \cdot < B \cdot \{A, H\} > \tag{1.1}$$

with A, B local observables (without loss of generality: real, differentiable functions with compact spatial support on phase space), H the Hamiltonian, β inverse temperature, $< \cdot >$ the thermal average and the Poisson bracket given by

$$\{A, B\} = \sum_i (\partial_{r_i} A \cdot \partial_{p_i} B - \partial_{p_i} A \cdot \partial_{r_i} B) \tag{1.2}$$

(1.1) was already derived by Mermin (cf. ref. [10]) and was used by him to get the classical counterpart of the so-called Bogoliubov inequality

$$< \{A, B\} >^2 \leq \beta < A^2 >< \{B, \{B, H\}\} > \tag{1.3}$$

which underlies, in various disguises, some of the approaches developed e.g. in the above cited papers.

On the other side there exists a considerable amount of model systems in classical statistical mechanics which do not openly carry such a nice structure, to mention typical cases in point, systems living on a discrete base-manifold as e.g. spin systems or systems defined via functional integrals.

In view of the great calculational advantages of the Poisson bracket formalism in classical statistical mechanics it would be highly desirable to have an analogous machinery at ones disposal for such (non-canonical) systems.

The necessary general steps in this direction have been undertaken by us in ref. [11]. Furthermore we studied a (however rather limited) class of models (e.g. interface Hamiltonian) to demonstrate the usefulness of our approach but made no systematic analysis of more complicated classes of spin systems which, while being of genuine relevance in statistical mechanics as such, serve furthermore as the starting point of Euclidean quantum field theory.

That is, we will derive in the following in a more systematic manner various (possibly new) classes of correlation (in)equalities for spin systems and apply them to typical problems in this field.

2. The Basic Estimates

In this chapter we will apply our general results ([11]) to spin systems. Furthermore, to keep matters transparent, we will treat, in a first step, continuous spin systems, i.e. each spin $S(x),\ x \in \mathbf{Z}^d$, ranges from plus to minus infinity.

This is a sufficiently large class of models being frequently discussed in the literature. Our formalism can of course also be applied to spins living on, say, a compact manifold as e.g. S^n etc.

In that particular case the independent variables defining the configuration space would be certain angles. With $\{S(x)\} = \mathbf{R}$ the technical manipulations are a little bit simpler (for a discussion of e.g. the $x-y-$model along these lines cf. [11]).

2.1 Remarks: i) One can, at least in principle, get corresponding results for constrained spin systems as limiting cases by approximating their support, e.g. given by $\delta(S^2-1)\cdot dS, S \in \mathbf{R}^d$, with the help of a sequence of smeared out distributions, taken from som function space, $\rho_n(S^2-1)$, which converge in this limit towards $\delta(S^2-1)$.

ii) Technically it turns out to be advantageous to absorb a possible extra weight function $\rho(S)$ occurring in the single-spin distribution into the Hamiltonian by writing it as an exponential.

With the base space being $\mathbf{Z}^d$ or $a\cdot\mathbf{Z}^d, a$, the lattice spacing, statistical mechanics on a subset $\Lambda \subset \mathbf{Z}^d$ is defined in the usual way via a Hamiltonian $H(\underline{S}), \underline{S} := \{S(x_i)\}, x_i \in \Lambda$, i.e.:

$$\begin{aligned} < A > &:= Z^{-1}\cdot\int A(\underline{S})e^{-\beta H(\underline{S})}d\underline{S} \\ \text{with } d\underline{S} &:= \Pi_{x_i\in\Lambda}dS(x_i), \\ Z &:= \int e^{-\beta H(\underline{S})}d\underline{S} \end{aligned} \tag{2.1}$$

(possible extra weight factors being absorbed in $H(\underline{S})$!).

As to the class of admissible observables we choose them to be real, differentiable functions with respect to the variables $S(x_i)$ and, if necessary, bounded away from the internal and (or) external system boundaries in order to avoid artificial boundary terms in the various partial integrations. This is however only a measure of precaution since, typically, at the internal system boundaries they are strongly supressed in most cases by the exponential vanishing of $exp(-\beta H)$ for some $S(x)$ approaching $\pm\infty$.

Now, as symmetries induced by Poisson brackets are locally generated by certain first order partial differential operators, we generalize the Poisson bracket structure of classical point mechanics by replacing Poisson brackets with general first order differential operators acting on the spins in the following way:

2.2 Definition: A first order differential operator operating on the spin system is given by

$$\mathcal{D} := \sum_i d_i(S_i)\partial_{S_i} \tag{2.2}$$

with d_i certain twice differentiable functions of the spin variable S_i (S_i abbreviation for $S(x_i)$), ∂_{S_i} denoting partial differentiation with respect to S_i. $\mathcal{D}$ is acting on observables, introduced above, i.e. on certain differentiable functions of the spins $\{S_i\}$.

2.3 Remark: Note that the d_i's can in principle carry an extra dependence on the site i, where they are localized.

With the help of such $\mathcal{D}$'s we are able to generalize the KMS-condition (1.1).

2.4 Generalized KMS-Condition:

$$\begin{aligned} < \mathcal{D}A > &= < A \cdot (\beta \mathcal{D}H - \text{ div } \underline{d}) > \\ \text{with div } \underline{d} &:= \sum_i \partial_{S_i} d_i(S_i) \end{aligned} \tag{2.3}$$

and after some calculations the Bogoliubov inequality (1.2).

2.5 Generalized Bogoliubov Inequality:

$$< \mathcal{D}A >^2 \leq < A >^2 \cdot < \beta \cdot \mathcal{D}\mathcal{D}H - \mathcal{D}(\text{ div } \underline{d}) > \tag{2.4}$$

2.6 Remarks: i) That these are the proper extensions of the relations (1.1), (1.2) to lattice systems has been shown in [11].

ii) We have given another, slightly different extension in [11] via augmenting the local phase space at each site x_i and the Hamiltonian H by means of which we get a true Poisson bracket structure also on the lattice.

Similar formulas can be derived for spin systems defined over a continuous base space, i.e. Euclidean quantum field theory over $\mathbf{R}^d$, where expectation values like (2.1) are replaced by functional integrals and the derivative operator $\mathcal{D}$ by a functional derivative:

$$< A >:= Z^{-1} \cdot \int D[\phi] A[\phi] e^{-\beta H[\phi]} \tag{2.5}$$

$D[\phi]$ being the functional measure, $H[\phi]$ the Euclidean action

$$\mathcal{D} := \int d^d x \; d(x, \phi(x)) \cdot \delta / \delta \phi(x) \tag{2.6}$$

(cf. [11]).

As one has to cope in this continuum situation with various renormalisation problems if one does not treat the expressions in a purely formal manner we plan to study this situation in a more systematic way in forthcoming work. On the other hand one can try to carry over the corresponding expressions from the lattice situation by taking the lattice spacing to zero.

2.7 Remark: In Euclidean field theory a certain method has been in use which bears a weak resemblance to our approach and which is called "The Integration by Parts Method". (cf. e.g. [12]). Our method however appears to be considerably more general and yields stronger results since it draws on concepts which have not been exploited up to now in that field.

3. Correlation Inequalities for the ϕ^4-System

The typical regime of application of relations of the above type is the important field of phase transitions and spontaneous symmetry breaking (examples can be found in the above mentioned literature).

In that situation the derivative operator $\mathcal{D}$ is typically chosen to be the generator of the flow representing the continuous "formal" symmetry of the model. The attribute "formal" means that in case the symmetry is spontaneously broken the Hamiltonian H is only invariant under the symmetry in a restricted (formal) sense and the manipulation of various limiting procedures becomes a highly delicate matter.

In the following we want to show that, perhaps a little bit surprisingly, the above formulas can be applied also in a much more general environment, e.g. where no continuous symmetry exists at all or where the symmetry is unbroken.

In this wider context the differential operator $\mathcal{D}$ does **not** suggest itself but has to be chosen cleverly in order to yield interesting (in)equalities between various expectation values or correlation functions.

3.1 Remark: In the following we will choose the differential operator $\mathcal{D}$ in such a way that div $\mathcal{D} \equiv 0$ holds in formulas (2.3), (2.4).

To begin with we take as model Hamiltonian the ϕ^4-Hamiltonian ($J_{ii} \equiv 0$) :

$$H = 1/2 \sum_{ij} J_{ij} S_i S_j + \sum_i m \; S_i^2 + \lambda \sum_i S_i^4 \tag{3.1}$$

and discuss this model for various choices of the parameters.

As interesting and more generic phenomena arise in the thermodynamic limit $\Lambda \longrightarrow \mathbf{Z}^d$ the following estimates are understood in this limit, i.e. they are calculated for finite Λ and are then generalized to the infinite system by a standard procedure.

The different classes of estimates arise from different choices of the observable A and operator $\mathcal{D}$ in formulas (2.3), (2.4). The limiting equilibrium state is assumed to represent a "pure phase". This can be achieved in the usual way by adding a symmetry breaking term in H which is switched off in the end or by fixing certain boundary conditions. As both A and $\mathcal{D}$ are chosen to be local, i.e. among other things, supported away from the system boundaries, there remains no explicit effect of these boundary conditions "at infinity".

3.2 The Case $A := S_i, \mathcal{D} := \partial_{S_i}$

Inequality (2.4) yields the estimate

$$1 = < 1 > \leq \beta < S_i^2 > \cdot (2m + 12\lambda \cdot < S_i^2 >) \tag{3.2}$$

with the Hamiltonian (3.1).

Solving for $< S_i^2 >$ we get:

i) $m \geq 0$:

$$< S_i^2 > \geq \frac{\sqrt{\frac{12\lambda}{\beta} + m^2} - m}{12\lambda} \tag{3.3}$$

ii) $m = 0$:

$$< S_i^2 > \geq \sqrt{\frac{1}{\beta \cdot 12\lambda}} \tag{3.4}$$

iii) $m > 0, \lambda \longrightarrow 0$:

$$< S_i^2 > \geq \frac{1}{2m\beta} \tag{3.5}$$

iv) $m < 0$ (i.e. ground state degenerated):

From (3.2) we infer:

$$\beta^{-1} \leq 12\lambda \cdot (< S_i^2 > + \frac{m}{12\lambda})^2 - \frac{m^2}{12\lambda} \tag{3.6}$$

and

$$2m + 12\lambda < S_i^2 > > 0 \qquad \text{always} \tag{3.7}$$

which yields

$$< S_i^2 > > -\frac{m}{6\lambda} \qquad \text{always} \tag{3.8}$$

Inserting this in (3.6) we see that the bracket is always positive also for $m < 0$!, i.e. there is no problem with the squareroot and we get, as in the case $m > 0$:

$$< S_i^2 > \geq \frac{\sqrt{\frac{12\lambda}{\beta} + m^2} - m}{12\lambda}, \qquad m < 0 \tag{3.9}$$

3.3 Remark: Note that our estimates hold both for the case $< S_i >= 0$ and $< S_i > \neq 0$, i.e. with or without spontaneous magnetization. That is, $< S_i^2 >$ is either a pure fluctuation term or contains the overall magnetization $< S_i >$.

As an application of our above estimates we will study the case $m < 0$ more closely. This is the regime where spontaneous symmetry breaking becomes possible. It is then an important question for which values of the phase space parameters, e.g. $\{\beta, m, \lambda\}$ the equilibrium state of the system represents the non-degenerated phase (i.e. single phase region) and for what values the equilibrium state is degenerated (i.e. two pure phases).

3.4 Remark: At the moment the relation of our results (presented below) to other kinds of estimates of these bounds (see e.g. [12]) is not entirely clear to us since they are usually derived by completely different methods. This point shall be clarified in the future.

We now study the particular model Hamiltonian

$$\begin{aligned} H &= \frac{1}{2} \sum_{nn} J \cdot (S_i - S_k)^2 + \sum_i (m_o S_i^2 + \lambda S_i^4), \quad J > 0 \\ &= -\sum_{nn} J \cdot S_i S_k + \sum_i (m S_i^2 + \lambda S_i^4) \end{aligned} \tag{3.10}$$

with $m := m_o + n \cdot J, n =$ number of nearest neighbors.

For $m_0 < 0, J \geq 0$, i.e. ferromagnetic coupling, the ground state ($\beta = \infty$), has $\overline{S} = \pm\sqrt{\mid m_0 \mid /2\lambda}$. With the help of our estimate for $< S_i^2 >$ we can provide a lower bound of the strength of fluctuation of S_i and can set it into relation to the inverse temperature β. That is:

$$\begin{aligned} < S_i^2 > -\overline{S}^2 &\geq \overline{S}^2 && \text{implies} \\ < (S_i - < S_i >)^2 > &\geq \overline{S}^2 = \frac{\mid m_0 \mid}{2\lambda} && \text{for } 0 \leq \mid < S_i > \mid \leq \mid \overline{S} \mid . \end{aligned} \tag{3.11}$$

We can now estimate the critical value for β so that the mean deviation from the average $< S_i >$ becomes larger than $\mid < S_i > \mid$ or $\mid \overline{S} \mid$ itself. We conjecture that this signals the transition from the two phase to the one phase regime as typical fluctuations will then connect the two minima. (We, however, do not intend to prove this at this place).

¿From (3.9) we get:

3.5 Observation: (3.11) holds if

$$\beta \leq \frac{\lambda}{14m_0^2 - 2nJ \cdot \mid m_0 \mid} =: \beta^* \qquad (\text{ and if } \beta^* > 0!) \tag{3.12}$$

i.e. we suppose that for $\beta \leq \beta^*$ the system is in the one-phase regime.

3.6 The Case $A := S_i \cdot S_j, \mathcal{D} = \partial_{S_j}$

Inserting these expressions into (2.4) yields:

$$< S_i >^2 \leq \beta < S_i^2 \cdot S_j^2 > (2m + 12\lambda < S_j^2 >) \tag{3.13}$$

If the system is in a pure state one can exploit well-known cluster theorems (cf. e.g. [13]) to infer:

$$< S_i^2 \cdot S_j^2 > \longrightarrow < S_i^2 > \cdot < S_j^2 > = < S_i^2 >^2 \quad \text{for } \mid i - j \mid \to \infty \tag{3.14}$$

This yields:

$$< S_i >^2 \leq \beta(2m < S_i^2 >^2 + 12\lambda < S_i^2 >^3) \tag{3.15}$$

and for $m < 0$:

$$< S_i^2 > \geq \left(\frac{< S_i >^2}{\beta \cdot 12\lambda} \right)^{1/3} \tag{3.16}$$

3.7 The Case $A := S_i^2 \cdot S_j, \mathcal{D} = \partial_{S_j}$

$$< S_i^2 >^2 \leq \beta \cdot < S_i^4 \cdot S_j^2 > \cdot (2m + 12\lambda < S_j^2 >) \tag{3.17}$$

and with the cluster property:

$$< S_i^4 > \geq \frac{< S_i^2 >}{\beta(2m + 12\lambda < S_i^2 >)} \tag{3.18}$$

It is evident that one can derive, proceeding in the indicated manner, a whole sequence of inequalities between various expectation values and correlation functions.

3.8 Remarks: i) Up to now our estimates are in general independent of the strength of the ("kinetic") coupling J_{ij}. This is a consequence of the choice ∂_{S_i} for $\mathcal{D}$. For $\mathcal{D} = \partial_{S_i} + \partial_{S_j}, i \neq j$. $\mathcal{D}\mathcal{D}H$ yields also terms containing the couplings J_{ij}.

ii) Furthermore, our results are dimension independent. This is, however, not always a disadvantage. The dependence on the space dimension has, on the other side, been exploited in previous work of us (cited above). To incorporate dimension one has to choose observables A which go with the volume Λ. In this paper A was fixed independent of Λ.

3.9 A Certain Strategy:

Our estimates yield bounds from below, i.e., as a case in point:

$$< S^2 > \geq \text{ expression (1) in } (\beta, m, \lambda) \tag{3.19}$$

If it is possible to derive a bound of the sort:

$$< (S - < S >)^2 > \; < \text{ expression (2) in } (\beta, m, \lambda) \tag{3.20}$$

it may become possible to get interesting bounds of the kind:

$$< S > \neq \; 0 \qquad \text{for a certain regime of } (\beta, m, \lambda) \tag{3.21}$$

i.e. estimates concerning the existence of phase transitions.

3.10 Observation: Note that estimate (3.8) is even independent of the inverse temperature β, i.e.

$$< S_i^2 > > \frac{\mid m \mid}{6\lambda} \qquad \text{for } m < 0 \tag{3.22}$$

This implies that in the limit $\beta \to \infty$ we end up in a completely ordered phase, i.e. spins aligned, or, in the cases where an ordered phase is excluded by e.g. Mermin-Wagner-theorem, the ground state consits of a random occupation of the two minima of the Hamiltonian.

In closing this paper we would like to point to the fact that up to now we have only exploited the inequality (2.4). Inserting, on the other side, the various choices for $A, \mathcal{D}$ into (2.3) we get an equality between certain expectation values. For the simplest choice, i.e.:

3.11 The Case $A := S_i, \mathcal{D} := \partial_{S_i}$; Equation (2.3)

$$\beta^{-1} = < \sum_j J_{ij} S_i S_j + 2mS_i^2 + 4\lambda S_i^4 > \tag{3.23}$$

which is reminiscent of sort of a virial theorem for spin systems. Corresponding equations can be derived for other choices of $A, \mathcal{D}$.

3.12 Remark: While we think the above scheme is representing a new approach to this

field it may well be that the results can possibly also be deduced by employing other methods. In any case, an advantage of our approach is, in our view, its simplicity and transparency.

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