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Griffiths Inequalities for Noninteracting N-Vector (Classical Heisenberg) Models and Applications to Interacting Systems

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An order relation for tensors is defined. With this ordering it is shown that in noninteracting N-vector models $\langle\sigma_A\sigma_B\rangle - \langle\sigma_A\rangle\langle\sigma_B\rangle$ is positive. Applications to interacting models include a proof for the alignment of spins and the subadditivity of the free energy.

KEY WORDS: N-vector model; spin system; correlation inequalities; free energy.

1. GENERALITIES

The second Griffiths inequality

$$\langle\sigma_A\sigma_B\rangle \geqslant \langle\sigma_A\rangle\langle\sigma_B\rangle, \qquad \sigma_A := \prod_{i\in A}\sigma_i \tag{1}$$

established originally[1,2] for the Ising model with ferromagnetic pair interactions (and special choices for A and B), has been generalized to Ising models with positive definite interactions[3] and to the 2-vector model (classical rotators, XY model).[4] In fact, proceeding from the Ising model (= 1-vector model) to N-vector models, the way to generalize (1) is not unique. Possible generalizations are, e.g., component inequalities and they are known to hold for $N \leqslant 4$ (see Ref. 5 for a review). The method which works for the componentwise inequalities is Ginibre's method of duplicating variables.[4] This method is explicitly known[6] to fail in the attempt to

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prove

$$\langle(\sigma_i \cdot \sigma_j)(\sigma_k \cdot \sigma_l)\rangle \geqslant \langle(\sigma_i \cdot \sigma_j)\rangle\langle(\sigma_k \cdot \sigma_l)\rangle \tag{2}$$

for N-vectors σ_i with $N \geqslant 3$.

An explicit counterexample to (2) for $N = 3$ is known in the quantum case,[7] but both the numerical studies by Sylvester[6] and the caricature of the N-vector model, in which the uniform measure on the sphere is replaced by the counting measure on the vertices of a cube,[7] support (2) in the classical case.

Even in models without interaction between the spins, (1) is not trivial. At least twice it has, however, been proved before, namely, by Ira Herbst with semigroup methods and by Loren D. Pitt with graphical methods[8] [for σ_A and σ_B monomials in $(\sigma_i \cdot \sigma_j)$].

We will proceed to prove in this setting the following somewhat stronger version:

Theorem. In the noninteracting N-vector model one has the inequality

$$\langle\sigma_A \otimes \sigma_B\rangle \succ \langle\sigma_A\rangle \otimes \langle\sigma_B\rangle \tag{3}$$

where σ_A and σ_B are tensors

$$\sigma_A = \bigotimes_{i \in A} \sigma_i\,, \qquad \sigma_B = \bigotimes_{i \in B} \sigma_i$$

A and B are ordered arrays of indices. Multiple appearance of indices is allowed. The order relation "$\succ$" [which will be formally defined in (12)] means that each contraction of all the tensor indices yields an ordinary inequality.

In contrast to (2) we allow here also contractions of indices in A with those in B. The index i denotes sites of a "lattice." The structure of this lattice is of course completely arbitrary, since $\langle\cdot\rangle$ denotes the integration with respect to the measure which is simply the product of the uniform and normalized measures on the surface of the N-spheres attached to each site.

We will first prove the theorem and then derive from it consequences for interacting systems. The Hamiltonians of these are supposed to be generalized ferromagnetic. By that we mean

$$-H \in \mathscr{F}_+$$

and

$$\mathscr{F}_+ := \left\{ f(\sigma) = \sum_{\substack{(A,B)\\ |A|=|B|}} \lambda_{AB} \prod_{\substack{i_k \in A\\ j_k \in B}} (\sigma_{i_k} \cdot \sigma_{j_k}),\ \lambda_{AB} \geqslant 0 \right\} \tag{4}$$

2. PROOF OF THE THEOREM

The advantage in taking first the expectations of tensorial quantities and the contractions afterwards, is that one can make use of "Wick's theorem" for the integral of products of the components of one spin $\sigma = \sigma_i$:

$$\text{(a)} \qquad \left\langle \prod_{k=1}^{2n+1} \sigma^{\alpha_k} \right\rangle = 0$$
$$\text{(b)} \qquad \left\langle \prod_{k=1}^{2n} \sigma^{\alpha_k} \right\rangle = \frac{1}{c(n)} \sum_{\text{pairings } \pi} \delta^{\pi} \tag{5}$$

Remark on the notation: Greek superscripts are used to denote the components of σ, π is a decomposition of $\{\alpha_1 \ldots \alpha_{2n}\}$ into pairs $\{\alpha_{i_1}, \alpha_{i_2}\} \cdots \{\alpha_{i_{2n-1}}, \alpha_{i_{2n}}\}$ and

$$\delta^{\pi} = \prod_{l=1}^{n} \delta^{\alpha_{i_{2l-1}} \alpha_{i_{2l}}}, \qquad c(n) = \prod_{k=0}^{n-1} (N + 2k) \tag{6}$$

This formula is well-known to the specialists,[6] but a proof does not seem to be readily available:

Proof. (a) is immediate from the symmetry $\sigma \to -\sigma$, (b) follows from Wick's theorem for Gaussian measures,[9] by considering a point $x \in \mathbb{R}^N$ in the representation $x = (\sigma, r)$, $r = |x|$, $\sigma = x/|x|$. (5b) is then the angular part of the integral $\int \prod_k x^{\alpha_k} \exp(-|x|^2/2)\, d^N x$. Evaluation of the radial part provides the factor $c(n)$. ■

For short hand notation we will use the inner product between tensors of the same rank:

$$(s, t) := \sum_{\alpha_1 \ldots \alpha_n} s^{\alpha_1 \ldots \alpha_n} t^{\alpha_1 \ldots \alpha_n} \tag{7}$$

We define an operator C, mapping tensors of rank $n+2$ to tensors of rank n:

$$(Ct)^{\alpha_1 \ldots \alpha_n} := \sum_{\beta, \gamma} \delta^{\beta\gamma} t^{\beta\gamma\alpha_1 \ldots \alpha_n}$$

Furthermore we denote by $\mathscr{P}_n$ the set of all permutation operators acting by permutation of n indices.

To motivate the definition (8) we remark that the contraction of all the indices of a tensor can of course be achieved by taking the inner product with a δ^{π}, and the corresponding alternative form of (3) is

$$(\delta^{\pi}, \langle \sigma_A \sigma_B \rangle) \geqslant (\delta^{\pi}, \langle \sigma_A \rangle \langle \sigma_B \rangle) \tag{3'}$$

We observe that all the tensors appearing in (3′) can be expressed in terms of the δ^{π}. We can thus restrict our attention to the corresponding subspace

$\mathscr{I}$ of tensors. Our strategy is then to consider the cone $\mathscr{I}_+$ generated by the δ^π and to show that $\langle\sigma_A\sigma_B\rangle - \langle\sigma_A\rangle\langle\sigma_B\rangle$ is an element of the dual cone $\mathscr{I}^+$.

Definition.

$$\mathscr{I}_+(2n) := \left\{ \sum_{\substack{\text{pairings } \pi \\ \text{of } 2n \text{ indices}}} \lambda_\pi \delta^\pi : \lambda^\pi \geqslant 0 \right\}, \qquad \mathscr{I}_+(2n+1) = \{0\},$$
$$\mathscr{I} = \mathscr{I}_+ - \mathscr{I}_+ \tag{8}$$

For $s \in \mathscr{I}_+$ we write also $s \geqslant 0$, for $s - t \in \mathscr{I}_+$ we write $s \geqslant t$.

Remark. We use the letter $\mathscr{I}$, because a $t \in \mathscr{I}$ is invariant under actions of the orthogonal group $O(N)$. We drop the indication of the rank, wherever it is not necessary. The following properties of $\mathscr{I}$ and $\mathscr{I}_+$ are obvious:

Lemma.

$$\begin{aligned}
&\text{(a)} \qquad \mathscr{I}_+(m) \otimes \mathscr{I}_+(n) \subset \mathscr{I}_+(m+n), \\
&\qquad\qquad \mathscr{I}(m) \otimes \mathscr{I}(n) \subset \mathscr{I}(m+n) \\
&\text{(b)} \qquad \forall P \in \mathscr{P}_n : P\mathscr{I}_+(n) = \mathscr{I}_+(n), \qquad P\mathscr{I}(n) = \mathscr{I}(n) \\
&\text{(c)} \qquad C\mathscr{I}_+(n+2) = \mathscr{I}_+(n), \qquad C\mathscr{I}(n+2) = \mathscr{I}(n) \\
&\text{(d)} \qquad (\mathscr{I}_+(n), \mathscr{I}_+(n)) \subset \mathbb{R}_+
\end{aligned} \tag{9}$$

From Wick's theorem, the product form of the free measure and (9a) there follows the following lemma.

Lemma.

$$\langle\sigma_A\rangle \geqslant 0 \tag{10}$$

As an aside we remark that the immediate consequence is the following

Griffiths' First Inequality. Let H be a generalized ferromagnetic Hamiltonian on a finite lattice. Then

$$\langle e^{-H}\sigma_A\rangle \geqslant 0 \tag{11}$$

Proof. By expansion of the exponential function we see that e^{-H} is in $\mathscr{I}_+$ [Eq. (4)]:

$$e^{-H} = \sum_C (t_C, \sigma_C), \qquad t_C \in \mathscr{I}_+$$

By virtue of (10)

$$\langle \sigma_C \otimes \sigma_A \rangle \in \mathscr{I}_+$$

and we may write

$$\langle (t_C, \sigma_C)\sigma_A \rangle = C^n P(t_C \otimes \langle \sigma_C \otimes \sigma_A \rangle) \in \mathscr{I}_+ \qquad \text{by lemma (9)}$$

with $C^n P$ contracting the indices of t_C with those of σ_C. ■

This result is in principle a known component inequality.[5] We now proceed with the proof of the theorem and define the dual cones.

Definition.

$$\mathscr{I}^+(n) := \{t \in \mathscr{I}(n) : \forall s \in \mathscr{I}_+(n) : (s,t) \geqslant 0\} \tag{12}$$

We write

$$\text{for} \quad t \in \mathscr{I}^+ : \qquad t \succ 0$$
$$\text{for} \quad t - s \in \mathscr{I}^+ : \qquad t \succ s$$

Because of (9d) we have

$$\mathscr{I}_+ \subset \mathscr{I}^+ \tag{13}$$

but $\mathscr{I}^+$ is strictly larger. As an example for a $t \in \mathscr{I}^+$ but $t \notin \mathscr{I}_+$, take

$$t^{\alpha\beta\gamma\delta} := -\delta^{\alpha\beta}\delta^{\gamma\delta} + \left[N(N+2)\right]^{-1}(\delta^{\alpha\beta}\gamma^{\gamma\delta} + \delta^{\alpha\gamma}\delta^{\beta\delta} + \delta^{\alpha\delta}\delta^{\beta\gamma})$$

This tensor originates as

$$\langle \sigma^\alpha \sigma^\beta \sigma^\gamma \sigma^\delta \rangle - \langle \sigma^\alpha \sigma^\beta \rangle \langle \sigma^\gamma \sigma^\delta \rangle$$

and we will eventually show that all expressions of this kind are elements of $\mathscr{I}^+$.

Since the δ^π form a basis of $\mathscr{I}_+$, an equivalent form of (12) is

$$t \in \mathscr{I}^+ \Leftrightarrow \forall \delta^\pi : (\delta^\pi, t) \geqslant 0 \tag{12'}$$

Lemma.

$$\begin{aligned}
&\text{(a)} \qquad \mathscr{I}_+(m) \otimes \mathscr{I}^+(n) \subset \mathscr{I}^+(m+n) \\
&\text{(b)} \qquad \forall P \in \mathscr{P}_n : P\mathscr{I}^+(n) = \mathscr{I}^+(n) \\
&\text{(c)} \qquad C\mathscr{I}^+(n+2) = \mathscr{I}^+(n)
\end{aligned} \tag{14}$$

Proof. (a) Let $s \in \mathscr{I}_+(m+n)$, $u \in \mathscr{I}_+(m)$, $t \in \mathscr{I}^+(n)$. Choose a permutation P such that

$$(s, u \otimes t) = (C^m P(s \otimes u), t)$$

The right-hand side is positive by Lemma (9) and by definition of $\mathscr{I}^+$, so (a) is proven.

(b) $(s, Pt) = (P^{\dagger} s, t) \geqslant 0$ where $P^{\dagger} = P^{-1}$ effects the inverse permutation.

(c) Let δ denote the Kronecker delta, and $s \in \mathscr{I}_{+}(n)$:

$$(s, Ct) = (\delta \otimes s, t) \geqslant 0 \qquad \text{since} \quad \delta \otimes s \in \mathscr{I}_{+}(n+2). \quad \blacksquare$$

A Counterexample. It is not true that $\mathscr{I}^{+} \otimes \mathscr{I}^{+}$ is a contained in $\mathscr{I}^{+}$. Take $t \in \mathscr{I}^{+}$:

$$t^{\alpha\beta\gamma\delta} = \delta^{\alpha\beta}\delta^{\gamma\delta} - N^{-1}\delta^{\alpha\gamma}\delta^{\beta\delta} \tag{15}$$

Contract $t^{\alpha\beta\gamma\delta}t^{\eta\epsilon\mu\nu}$ with $\delta^{\alpha\eta}\delta^{\beta\mu}\delta^{\gamma\epsilon}\delta^{\delta\nu}$. The result is $N^{-1} - N < 0$ for $N > 1$.

The crux of all this is now

Proposition.

$$\text{Let } s_k \geqslant 0,\ t_k \geqslant 0,\ s_k \succ t_k\text{, then } \bigotimes_{k=1}^{n} s_k \succ \bigotimes_{k=1}^{n} t_k \tag{16}$$

Proof. Write the difference of the products as a telescopic sum

$$\bigotimes_{k=1}^{n} s_k - \bigotimes_{k=1}^{n} t_k = \sum_{k=1}^{n} \left[\bigotimes_{j=1}^{k-1} s_j \right] \otimes (s_k - t_k) \otimes \left[\bigotimes_{j=k+1}^{n} t_j \right]$$

We have

$$s_k - t_k \succ 0$$

$$\bigotimes s_j \geqslant 0$$

$$\bigotimes t_j \geqslant 0$$

so each term in the sum is $\succ 0$. $\blacksquare$

Now we are in the position to prove the theorem

$$\langle \sigma_A \otimes \sigma_B \rangle \succ \langle \sigma_A \rangle \otimes \langle \sigma_B \rangle$$

Proof. (For the sake of simplicity, we write now the tensor product like an ordinary product.) Bring by a permutation P_1, σ_A into the form

$$\sigma_A = P_1 \prod_i \tau_i$$

where each τ_i collects all the factors σ_i from one site, so that $\langle \sigma_A \rangle = P_1 \prod_i \langle \tau_i \rangle$. Similarly

$$\sigma_B + P_2 \prod_i \rho_i, \qquad \langle \sigma_B \rangle = P_2 \prod_i \langle \rho_i \rangle$$

By permuting the indices again, let

$$\langle \sigma_A \sigma_B \rangle = P \prod_i \langle \tau_i \rho_i \rangle$$

and

$$\langle \sigma_A \rangle \langle \sigma_B \rangle = P \prod_i \langle \tau_i \rangle \langle \rho_i \rangle$$

so that

$$\langle \sigma_A \sigma_B \rangle - \langle \sigma_A \rangle \langle \sigma_B \rangle = P\Big(\prod_i \langle \tau_i \rho_i \rangle - \prod_i \langle \tau_i \rangle \langle \rho_i \rangle \Big)$$

Now we have the situation of proposition (16), since

$$\langle \tau_i \rangle \langle \rho_i \rangle \geqslant 0, \qquad \langle \tau_i \rho_i \rangle \geqslant 0$$

It remains to show that

$$\langle \tau_i \rho_i \rangle \succ \langle \tau_i \rangle \langle \rho_i \rangle$$

This is trivial if τ or ρ contain an odd number of components of σ, so we assume both to be even. Since $\mathscr{T}_+$ is spanned by tensors δ^π, we have to show that for any pairing π

$$(\delta^\pi, \langle \tau\rho \rangle) \geqslant (\delta^\pi, \langle \tau \rangle \langle \rho \rangle) \tag{17}$$

Remember that $\tau^{\alpha\beta\cdots} = \sigma^\alpha \sigma^\beta \ldots$ with $\sigma^2 = 1$. You see that in the left-hand side

$$\langle (\delta^\pi, \tau\rho) \rangle = \Big\langle \prod \sigma^2 \Big\rangle = 1$$

and the right-hand side is of the form

$$\sum_{\alpha_1 \ldots \alpha_n} \langle \sigma^{\alpha_1} \sigma^{\alpha_2} \cdots \sigma^{\alpha_n} \rangle \langle \sigma^{\alpha_1} \sigma^{\alpha_2} \cdots \sigma^{\alpha_n} \rangle = \frac{1}{c(n/2)} \tag{18}$$

as is obvious applying Wick's theorem to one of the factors and again using

$$\Big\langle \Big(\delta^\pi, \prod \sigma \Big) \Big\rangle = 1$$

Now remember that $c(n) \geqslant 1$ and the theorem is proven. ■

3. APPLICATIONS TO INTERACTING SYSTEMS

We indicate the free measure now by $\langle\ \rangle_0$.

Corollary 1. Let H be a generalized ferromagnetic Hamiltonian, let

$$\langle \sigma_A \rangle_H := \langle e^{-H} \rangle_0^{-1} \langle \sigma_A e^{-H} \rangle_0$$

Then

$$\langle \sigma_A \otimes \sigma_B \rangle_H \succ \langle \sigma_A \rangle_H \otimes \langle \sigma_B \rangle_0 \tag{19}$$

Proof. The proof proceeds from the theorem in the same way, as the proof of (11) proceeds from the Lemma (10), namely, by expansion of e^{-H} on both sides and by the use of the theorem for each term. ■

Example.

$$\langle (\sigma_i \cdot \sigma_j)(\sigma_i \cdot \sigma_k) \rangle_H \geqslant \sum_{\alpha, \beta} \langle \sigma_j^\alpha \sigma_k^\beta \rangle_H \langle \sigma_i^\alpha \sigma_i^\beta \rangle_0 = N^{-1} \langle \sigma_j \cdot \sigma_k \rangle_H \tag{20}$$

For a system in an external magnetic field, we can apply the method of the "ghost spin", i.e., think of σ_i as generating the magnetic field.[2] Let e be the unit vector in the direction of the field. You get

$$\langle (\sigma_j \cdot e)(\sigma_k \cdot e) \rangle_H \geqslant N^{-1} \langle (\sigma_j \cdot \sigma_k) \rangle_H \tag{21}$$

This means that in the presence of an external magnetic field the components of the spin in the field direction are stronger correlated than the other components. They are also stronger correlated than in the absence of the field, because, in this case, the both sides of (21) would be equal in magnitude.

If we set $\sigma_A = 1$ in (19), we obtain

Corollary 2. For H generalized ferromagnetic

$$\langle \sigma_B \rangle_H \succ \langle \sigma_B \rangle_0 \tag{22}$$

If one contracts the indices, this is the inequality

$$\left\langle \prod_{(j,k)} (\sigma_{i_j} \cdot \sigma_{i_k}) \right\rangle_H \geqslant \left\langle \prod_{(j,k)} (\sigma_{i_j} \cdot \sigma_{i_k}) \right\rangle_0 \tag{23}$$

This inequality shows that a ferromagnetic interaction favors the alignment of spins. It is in some sense stronger than what is usually called the first Griffiths inequality, which implies only

$$\left\langle \prod_{(j,k)} (\sigma_{i_j} \cdot \sigma_{i_k}) \right\rangle_H \geqslant 0 \tag{24}$$

As an example for the difference between (23) and (24) consider the special case of (23)

$$\langle (\sigma_i \cdot \sigma_j)^2 \rangle_H \geqslant 1/N \tag{25}$$

For $N = 1$, the right-hand side of (23) is only in those cases not equal to zero, where the variable is identical equal to one, so the content of (23) and (24) is the same. But for higher "spin"-dimensions, (23) is stronger, and it is only this inequality which generalizes the first Griffiths inequality with respect to its meaning, namely, the alignment of spins.

While (21) and (23) are confirmations of intuitively obvious facts, the following statement is less intuitive. It shows that generalized ferromagnetic Hamiltonians are the analog of purely attractive interactions.

Corollary 3. The canonical free energy

$$F(\beta, H) := -\beta^{-1}\log\langle e^{-\beta H}\rangle_0$$

is negative and subadditive on the space of generalized ferromagnetic Hamiltonians:

$$F(\beta, H + K) \leqslant F(\beta, H) + F(\beta, K) \tag{26}$$

Proof. One has to show $\langle e^{-\beta H}\rangle_0 \geqslant 1$ and

$$\langle e^{-\beta(H+K)}\rangle_0 \geqslant \langle e^{-\beta H}\rangle_0 \langle e^{-\beta K}\rangle_0$$

This follows again by expansion of the exponentials and termwise application of the Lemma (10) and of the theorem. ■

Now consider disjoint volumes (= sets of sites) V and W. Let the respective Hamiltonians be H_V and H_W, and let K be the interaction between V and W, so that

$$H_{V \cup W} = H_V + H_W + K$$

Suppose that all these Hamiltonians are generalized ferromagnetic. Then (26), $\langle e^{-\beta K}\rangle_0 \geqslant 1$ and

$$\langle e^{-\beta(H_V + H_W)}\rangle_0 = \langle e^{-\beta H_V}\rangle_0 \langle e^{-\beta H_W}\rangle_0$$

imply the subadditivty of the free energy as function of the volume:

Corollary 4.

$$F(\beta, H_{V \cup W}) \leqslant F(\beta, H_V) + F(\beta, H_W) \tag{27}$$

As is well known, this subadditivity is useful to obtain a simple proof for the existence of the thermodynamic limit.[10]

Since dimensional analysis is simportant in statistical mechanics and field theory, we add the following result:

Corollary 5. Let V_n be the n-dimensional simple cubic lattice $L \times L \times \cdots \times L$, with $L = \{1, 2, \ldots, l\}$. Let H_n be the Hamiltonian $H_n =$

$-\lambda\sum_{\langle i,j\rangle}(\sigma_i \cdot \sigma_j)$, where the sum is over all pairs of nearest neighbors. Then the free energy per site,

$$f(\beta, H_n) = l^{-n}F(\beta, H_n, V_n) \tag{28}$$

(we indicate here explicitly the lattice in which H_n is supposed to act) is a decreasing and subadditive function of the lattice dimension n:

$$f(\beta, H_{m+n}) \leqslant f(\beta, H_m) + f(\beta, H_n) \tag{29}$$

(The spin dimension is kept fixed.)

Proof. Observe that

$$V_{m+n} = V_m \times V_n \tag{30}$$

and

$$H_{m+n} = H_m + H_n \tag{31}$$

where H_m acts in the first, and H_n in the second factor of (30), i.e., H_m collects all the interactions along links which are parallel to the m first coordinate directions, H_n the other ones along the links which are parallel to the n last coordinate directions.

For the single summand in (31) we have

$$F(\beta, H_m, V_{m+n}) = l^n F(\beta, H_m, V_m)$$

We use this on the right-hand side of (26) with H_{m+n} taking the role of $H + K$:

$$F(\beta, H_{m+n}, V_{m+n}) \leqslant l^n F(\beta, H_m, V_m) + l^m F(\beta, H_n, V_n)$$

Division by l^{m+n} yields the desired result. ■

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