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GKS Inequalities for Arbitrary Spin Ising Ferromagnets

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Elementary proofs of the first and second Griffiths–Kelly–Sherman (GKS) inequalities are given for higher-spin Ising systems with a Hamiltonian containing only a quadratic form in the spin variables and integer powers of single spin variables. These proofs are obtained using Gaussian random variables. A slight generalization of previous results has been obtained in that the coefficients of the even powers of the spin variables are allowed to be negative.

KEY WORDS: Ising spin systems; Griffiths, Kelly, Sherman inequalities; Gaussian random variables.

1. INTRODUCTION

For a system of N Ising spins attached to points of a lattice Ω, the Griffiths–Kelly–Sherman (GKS) inequalities[1] state that

$$\left\langle \prod_{i\in A} \sigma_i \right\rangle \geqslant 0 \tag{1}$$

and

$$\left\langle \prod_{j\in B} \sigma_j \prod_{k\in C} \sigma_k \right\rangle - \left\langle \prod_{j\in B} \sigma_j \right\rangle \left\langle \prod_{k\in C} \sigma_k \right\rangle \geqslant 0 \tag{2}$$

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where σ_i, σ_j, $\sigma_k = \pm 1$ are Ising spin variables associated with the points i, j, and k of Ω, and A, B, and C are subsets of Ω. The bracket $\langle\ \rangle$ denotes the average in the canonical ensemble[2] with Hamiltonian

$$H = -\sum_{A \subset \Omega} J_A \prod_{i \in A} \sigma_i \tag{3}$$

where J_A is required to be nonnegative for all $A \subset \Omega$. These inequalities have been generalized to the case of systems having spin variables s_i, where $s_i = p, p-2, \ldots, -p+2, -p$, and to products of spin variables

$$s^\delta \equiv \prod_{i=1}^{N} (s_i)^{\delta_i} \tag{4}$$

where δ_i is a multiplicity function assigning to each site $i \in \Omega$ a nonnegative integer. The inequalities then become

$$\langle s^\delta \rangle \geqslant 0 \tag{5}$$

and

$$\langle s^\delta s^\nu \rangle - \langle s^\delta \rangle \langle s^\nu \rangle \geqslant 0 \tag{6}$$

for systems with the general Hamiltonian

$$H = -\sum_\mu J_\mu s^\mu \tag{7}$$

with the restriction $J_\mu \geqslant 0$ for all μ.[2]

We present here a rather simple proof of the inequalities (5) and (6), using the method of random variables, for the case of the higher-spin systems with Hamiltonian

$$H = -\tfrac{1}{2} \sum_{i \neq j} J(i,j) s_i s_j - \sum_{\substack{m \\ \text{odd}}} h_m \sum_{i=1}^{N} (s_i)^m - \sum_{\substack{n \\ \text{even}}} \mu_n \sum_{i=1}^{N} (s_i)^n \tag{8}$$

where m and n are, respectively, odd and even positive integers, $J(i,j) \geqslant 0$ for all (i,j), $h_m \geqslant 0$ for all m, and $J(j,i) = J(i,j)$. The Hamiltonian (8) is more restricted than (7), for which (5) and (6) are valid in that the method of random fields restricts us to the pair interaction. However, while previous proofs of the inequalities have relied on first proving them for a spin-$\frac{1}{2}$ system and then, by use of Griffith's weight functions,[2] expressing the higher-spin systems in terms of spin-$\frac{1}{2}$ systems, the following method deals directly with the higher-spin systems. (The case of $s_i = \pm 1$ is presented separately in the following sections before the general spin case only for the purpose of first illustrating the proofs with a minimum of computational difficulties.) Also, in the previous proofs of the inequalities a necessary re-

[2] To be distinguished from the average $\langle\ \rangle_{Av\alpha}$ to be introduced later.

quirement was that all interaction coefficients be nonnegative. Here this restriction on the factors μ_n is dropped and these interactions can take on any value.

The method of random fields has been used by several authors[(3)] for the investigation of the neighborhood of the Weiss limit. It is based on the identity[(4)]

$$\exp\left[\tfrac{1}{2}\sum_{k,l}\xi_k\alpha_{kl}\xi_l\right] = (2\pi)^{-N/2}(\det\alpha)^{-1/2} \times \int\cdots\int\left\{\exp\left[-\tfrac{1}{2}\sum_{k,l}x_k(\alpha^{-1})_{kl}x_l + \sum \xi_j x_j\right]\right\}\prod_{i=1}^{N} dx_i \tag{9}$$

valid for any symmetric, real, and positive-definite matrix α, and for any N complex variables ξ_k. The sign of $(\det\alpha)^{-1/2}$ is to be chosen positive. The right-hand side of Eq. (9) can be considered as the average $\langle\exp\sum_{j=1}^{N} x_j\xi_j\rangle_{Av\alpha}$, where $\langle\ \rangle_{Av\alpha}$ denotes the average with respect to the probability density

$$W_N(\mathbf{x}) = (2\pi)^{-N/2}(\det\alpha)^{-1/2}\exp\left[-\tfrac{1}{2}\sum_{k,l=1}^{N} x_k(\alpha^{-1})_{kl}x_l\right] \tag{10}$$

where $\mathbf{x}$ is the vector with components x_j.

One derives from this easily the averages

$$\left\langle\prod_{j=1}^{N} x_{l_j}\right\rangle_{Av\alpha} = \begin{cases} 0 & \text{for } n \text{ odd} \\ \sum_{\text{pairings}}\prod\alpha_{st} & \text{for } n \text{ even}\end{cases} \tag{11}$$

where the numbers l_j are positive integers less than N, not necessarily distinct, and st are pairs of numbers l_j. The sum $\sum_{\text{pairings}}$ extends over all the different ways of dividing the numbers l_j into different pairs (st and ts are considered the same pair). For example, $\langle x_1x_2\rangle = \alpha_{12}$, $\langle x_1x_2{}^2x_4\rangle = 2\alpha_{12}\alpha_{24} + \alpha_{14}\alpha_{22}$, and $\langle x_1x_2x_3x_4\rangle = \alpha_{12}\alpha_{34} + \alpha_{13}\alpha_{24} + \alpha_{14}\alpha_{23}$. Clearly if all elements of α are nonnegative, then

$$\left\langle\prod_{j=1}^{N} x_j^{n_j}\right\rangle \geqslant 0 \tag{12}$$

where all n_j are nonnegative integers.[3]

The identity (9) can be used to rewrite the Boltzmann factor $e^{-\beta H}$, by identifying the variable ξ_j with the spin variables s_j and forming a matrix $J = \alpha$ with off-diagonal elements $J(i,j)$ and all diagonal elements equal to a number $J_0 \equiv J(i,i)$ large enough to guarantee that J is positive definite. The

[3] Leff[(5)] used this fact to prove GKS-type inequalities for oscillator coordinates.

Boltzmann factor with the Hamiltonian (8) and $\beta \equiv 1/kT$ is then

$$\exp -\beta H = \left\langle \exp \sum_{k=1}^{N} \left\{ \beta^{1/2} x_k s_k + \beta \sum_{\substack{m \\ \text{odd}}} h_m (s_k)^m + \beta \sum_{\substack{n \\ \text{even}}} \mu_n (s_k)^n - \tfrac{1}{2}\beta J_0 (s_k)^2 \right\} \right\rangle_{AvJ} \tag{13}$$

Here we only assumed J to be positive definite and $J(i,j)$ real and symmetric, $J(i,j) = J(j,i)$. Also, the dimensionality of the lattice Ω does not enter; in fact, Ω need not be a regular lattice, but any set of N points.

2. THE FIRST GKS INEQUALITY

The following restricted theorem for the spin-$\frac{1}{2}$ case is proven before the general theorem which follows.

Theorem 1′. For the case when $s_i = \pm 1$, $J(i,j) \geqslant 0$, and $h_1 \geqslant 0$ the following inequality is valid: $\langle s_i \rangle \geqslant 0$.

Proof. For the case of $s_i = \pm 1$ the terms μ_n and h_m with $m > 1$ are irrelevant. Therefore for the thermal average $\langle s_i \rangle$ one has from (8) and (13)

$$\begin{aligned} Z_N \langle s_i \rangle = {} & (2\pi)^{-N/2} (\det J)^{-1/2} [\exp(-\tfrac{1}{2} N J_0 \beta)] \\ & \times \sum_{\{s\}} \int \cdots \int d^N x \exp\left[-\tfrac{1}{2} \sum_{k,l} x_k (J^{-1})_{kl} x_l \right] \\ & \times [\partial / \partial (\beta^{1/2} x_i)] \exp\left[\beta^{1/2} \sum_{k=1}^{N} x_k s_k + \beta h \sum_{k=1}^{N} s_k \right] \end{aligned} \tag{14}$$

After the sum over configurations $\{s\}$ is carried out this becomes

$$\begin{aligned} Z_N \langle s_i \rangle = {} & (2\pi \exp \beta J_0)^{-N/2} (\det J)^{-1/2} \int \cdots \int d^N x \\ & \times \left\{ \exp\left[-\tfrac{1}{2} \sum x_k (J^{-1})_{kl} x_l \right] \right\} \\ & \times \left\{ [\partial / \partial (\beta^{1/2} x_i)] \prod_{k=1}^{N} 2 \cosh(\beta^{1/2} x_k + \beta h) \right\} \end{aligned} \tag{15}$$

It remains to show that the right-hand side of (15) is nonnegative. By taking the series expansion of the cosh terms and performing the partial differentiation, it is seen that the expression in the curly brackets becomes a summation of terms of the form $C(\alpha_1, \alpha_2, \ldots, \alpha_N) x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_N^{\alpha_N}$, where the α's are nonnegative integers and $C(\alpha_1, \alpha_2, \ldots, \alpha_N)$ is a nonnegative constant given that $h_1 \geqslant 0$. Therefore the r.h.s. of (15) is a sum of terms of the above form averaged with respect to the probability density (10), with α replaced by J. By (12) one has that the average of $x_1^{\alpha_1}x_2^{\alpha_2}...x_N^{\alpha_N}$ with respect to the probability density (10) is nonnegative given $J(i,k) \geqslant 0$ for all (i,j). Hence the r.h.s. of (15) is a sum of positive terms and the theorem is proven.

The general theorem follows:

Theorem 1. Given the Ising system of Section 1 with Hamiltonian (8), the following inequality holds

$$\langle s^\delta \rangle \geqslant 0 \tag{16}$$

whenever $J(i,j) \geqslant 0$ for all (i,j) and $h_m \geqslant 0$ for all m.

Proof. Calculation of the thermal average of s^δ using (8) and (13) after performing the summation over $\{s_i\}$ gives

$$\begin{aligned} Z_N\langle s^\delta\rangle = {}& (2\pi)^{-N/2}(\det J)^{-1/2} \int\cdots\int d^N x \exp\left[-\tfrac{1}{2}\sum_{k,l} x_k(J^{-1})_{kl}x_l\right] \\ & \times \prod_{i=1}^{N} [\partial^{\delta_i}/\partial(\beta^{1/2}x_i)^{\delta_i}]\left\{\sum_{s_i} \delta_{s_i,0}\right. \\ & \left. + \sum_{s_i>0} 2\left\{\exp\left[\beta\sum_n \mu_n(s_i)^n\right]\right\}\cosh\left[\beta^{1/2}x_is_i + \beta\sum_m h_m(s_i)^m\right]\right\} \end{aligned} \tag{17}$$

where the term J_0 has been included in the μ_2 term and the $\delta_{s_i,0}$ is the usual Kronecker delta. It should be noted that the cosh terms appear because of the fact that if $s_i = +q$, there is also the term $s_i = -q$ except for the case $s_i = 0$, which gives rise to the $\delta_{s_i,0}$. The proof now follows as before: After expansion of the cosh terms and differentiation, the right-hand side of (17) becomes a sum of terms of the form $C(\alpha_1, \alpha_2,..., \alpha_N)x_1^{\alpha_1}x_2^{\alpha_2}...x_N^{\alpha_N}$, where C is a positive constant, averaged with respect to the probability density (10) and hence positive.

3. THE SECOND GKS INEQUALITY

The second GKS inequalities are now proven beginning with the simplest inequality for the spin-$\frac{1}{2}$ system.

Theorem 2′. For the case where $s_i = \pm 1$, $J(i,j) \geqslant 0$, and $h_1 \geqslant 0$ the following inequality holds: $\langle s_is_j\rangle - \langle s_i\rangle\langle s_j\rangle \geqslant 0$.

Proof. As in Theorem 1′ for the case of $s_i = \pm 1$ the terms μ_n and h_m with $m > 1$ are redundant. Therefore for the above inequality one has from (8) and (13)

$$
\begin{aligned}
&Z_N{}^2[\langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle] \\
&\quad = (2\pi)^{-N}(\det J)^{-1}[\exp(-NJ_0\beta)] \sum_{\{s\}}\sum_{\{s'\}} \int\cdots\int d^N x\, d^N y \\
&\qquad \times \exp\Big[-\tfrac{1}{2}\sum_{k,l} x_k (J^{-1})_{kl} x_l\Big] \exp\Big[-\tfrac{1}{2}\sum_{k,l} y_k (J^{-1})_{kl} y_l\Big] \\
&\qquad \times \frac{\partial}{\partial(\beta^{1/2}x_i)}\Big[\frac{\partial}{\partial(\beta^{1/2}x_j)} - \frac{\partial}{\partial(\beta^{1/2}y_j)}\Big] \\
&\qquad \times \exp\Big\{\sum_{k=1}^{N} [\beta^{1/2}(s_k x_k + s_k' y_k) + \beta h(s_k + s_k')]\Big\} \qquad (18)
\end{aligned}
$$

Defining new variables

$$\eta_k = (1/\sqrt{2})(x_k + y_k), \qquad \xi_k = (1/\sqrt{2})(x_k - y_k) \qquad (19)$$

one can rewrite (18) as

$$
\begin{aligned}
&Z_N{}^2[\langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle] \\
&\quad = (2\pi)^{-N}(\det J)^{-1}[\exp(-NJ_0\beta)] \sum_{\{s\}}\sum_{\{s'\}} \int\cdots\int d^N \eta\, d^N \xi \\
&\qquad \times \exp\Big[-\tfrac{1}{2}\sum_{k,l} \eta_k (J^{-1})_{kl} \eta_l\Big] \exp\Big[-\tfrac{1}{2}\sum_{k,l} \xi_k (J^{-1})_{kl} \xi_l\Big] \\
&\qquad \times \Big(\frac{\partial}{\partial[(2\beta)^{1/2}\eta_i]} + \frac{\partial}{\partial[(2\beta)^{1/2}\xi_i]}\Big)\frac{\partial}{\partial[(\tfrac{1}{2}\beta)^{1/2}\xi_j]} \\
&\qquad \times \exp\Big\{\sum_{k=1}^{N} [\beta^{1/2}(s_k x_k + s_k' y_k) + \beta h(s_k + s_k')]\Big\} \qquad (20)
\end{aligned}
$$

Performing the summation over $\{s\}$ and $\{s'\}$ gives

$$
\begin{aligned}
&Z_N{}^2[\langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle] \\
&\quad = (2\pi)^{-N}(\det J)^{-1}[\exp(-NJ_0\beta)] \int\cdots\int d^N \eta\, d^N \xi \\
&\qquad \times \exp\Big[-\tfrac{1}{2}\sum_{k,l} \eta_k (J^{-1})_{kl} \eta_l\Big] \exp\Big[-\tfrac{1}{2}\sum_{k,l} \xi_k (J^{-1})_{kl} \xi_l\Big] \\
&\qquad \times \frac{1}{\beta}\Big(\frac{\partial}{\partial\eta_i} + \frac{\partial}{\partial\xi_i}\Big)\Big(\frac{\delta}{\partial\xi_j}\Big) \\
&\qquad \times \prod_{k=1}^{N} [2\cosh[(2\beta)^{1/2}\eta_k + 2\beta h] + 2[\cosh(2\beta)^{1/2}\xi_k] \qquad (21)
\end{aligned}
$$

As with the case of the first GKS inequality, the right-hand side, after expanding the cosh terms and taking the partial derivatives, is a sum of terms of the form

$$C(\alpha_1,\ldots, \alpha_N, \alpha_1{}',\ldots, \alpha_N{}')\eta_1^{\alpha_1}\cdots\eta_N^{\alpha_N}\xi_1^{\alpha_1{}'}\cdots\xi_N^{\alpha_N{}'}$$

with the constant C positive for $h_m > 0$. The η's and ξ's are averaged with respect to their respective Gaussian averages and again as in Theorem 1 these averages are positive. Hence the positivity of the right-hand side of (21) and the theorem is proven.

The general theorem for the second GKS inequality follows:

Theorem 2. Given the Ising spin system of Section 1 with Hamiltonian (8), the following inequality holds:

$$\langle s^\delta s^\nu\rangle - \langle s^\delta\rangle\langle s^\nu\rangle \geqslant 0 \tag{22}$$

whenever $J(i,j) \geqslant 0$ for all (i,j) and $h_m \geqslant 0$ for all m.

Proof. Using the new variables ξ_k and η_k of (19), one has

$$\begin{aligned}
&Z_N{}^2[\langle s^\delta s^\nu\rangle - \langle s^\delta\rangle\langle s^\nu\rangle] \\
&\quad = (2\pi)^{-N}(\det J)^{-1}\sum_{\{s\}}\sum_{\{s'\}}\int\cdots\int d^N\xi\, d^N\eta \\
&\qquad \times \exp\left[-\tfrac{1}{2}\sum_{k,l}\eta_k(J^{-1})_{kl}\eta_l\right]\exp\left[-\tfrac{1}{2}\sum_{k,l}\xi_k(J^{-1})_{kl}\xi_l\right] \\
&\qquad \times \prod_{i,j=1}^{N}\left\{\left[\frac{1}{(2\beta)^{1/2}}\right]^{\delta_i}\left(\frac{\partial}{\partial\eta_i}+\frac{\partial}{\partial\xi_i}\right)^{\delta_i}\left[\frac{1}{(2\beta)^{1/2}}\right]^{\nu_j}\right. \\
&\qquad \times \left[\left(\frac{\partial}{\partial\eta_j}+\frac{\partial}{\partial\xi_j}\right)^{\nu_j} - \left(\frac{\partial}{\partial\eta_j}-\frac{\partial}{\partial\xi_j}\right)^{\nu_j}\right]\exp[\beta^{1/2}(s_i x_i + s_i' y_i') \\
&\qquad \left.\left. + \beta\sum_{\substack{m\\ \text{odd}}} h_m((s_i)^m + (s_i')^m) + \beta\sum_{\substack{n\\ \text{even}}}\mu_n((s_i)^n + (s_i')^n)\right]\right\}
\end{aligned} \tag{23}$$

The remainder of the proof consists in rearrangement of the derivative terms and those terms involving s_i and s_i' to obtain the right-hand side of (23) as a sum of positive terms. First the negative terms of the derivatives cancel and give

$$\left(\frac{\partial}{\partial\eta_j}+\frac{\partial}{\partial\xi_j}\right)^{\nu_j} - \left(\frac{\partial}{\partial\eta_j}-\frac{\partial}{\partial\xi_j}\right)^{\nu_j} = 2\sum_{\substack{p\\ \text{odd}}}^{\nu_j}\frac{(\nu_j)!}{(\nu_j-p)!\,p!}\left(\frac{\partial}{\partial\eta_j}\right)^{\nu_j-p}\left(\frac{\partial}{\partial\xi_j}\right)^{p} \tag{24}$$

The terms containing s_i and s_i' can be written as

$$\begin{aligned}
&\sum_{s,s'}\exp\left\{\beta^{1/2}(sx + s'y) + \beta\sum_{\substack{m\\ \text{odd}}} h_m[(s)^m + (s')^m] + \beta\sum_{\substack{n\\ \text{even}}}\mu_n\,[(s)^n + (s')^n]\right\} \\
&\quad = \sum_{s,s'}\cosh\left[(\tfrac{1}{2}\beta)^{1/2}(s+s')\xi + \beta\sum_m h_m[(s)^m + (s')^m]\right] \\
&\qquad \times \cosh[(\tfrac{1}{2}\beta)^{1/2}|(s-s')|\eta]\exp\left\{\beta\sum_n \mu_n[(s)^n + (s')^n]\right\}
\end{aligned} \tag{25}$$

Therefore, as in the previous proofs, by using the series expansion of the cosh terms, if $h_m \geqslant 0$ for all m, then the right-hand side of (23) is a sum of terms of the form

$$C(\alpha_1,..., \alpha_N, \alpha_1',..., \alpha_N')\eta_1^{\alpha_1}\cdots\eta_N^{\alpha_N}\xi_1^{\alpha_1'}\cdots\xi_N^{\alpha_N'}$$

with $C(...) \geqslant 0$. The products of the variables ξ and η, averaged with respect to Gaussian probability densities in η and ξ, are positive if $J(i,j) \geqslant 0$ for all (i,j).

4. SUMMARY

Elementary proofs of the first and second GKS inequalities are presented for Ising models with the Hamiltonian

$$H(\{s\}) = -\tfrac{1}{2}\sum_{i\neq j} J(i,j)s_is_j - \sum_{\substack{m\\ \text{odd}}} h_m \sum_{i=1}^{N} (s_i)^m - \sum_{\substack{n\\ \text{even}}} \mu_n \sum_{i=1}^{N} (s_i)^n \qquad (26)$$

where $s_i = p,\ p-2,..., -p+2, -p, J(i,j) \geqslant 0$ for all pairs (i,j), and $h_m \geqslant 0$ for all m.[4] No positivity assumptions are needed for the factors μ_n. The proofs use the representation of the Boltzmann factor as an average over Gaussian random variables.

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[4] Note Added in Proof: The requirement that $h_m \geq 0$ for all odd m is a sufficient condition but not a necessary one, e.g., if $h_m = 0$ for all $m > 3$, one may allow $h_1 \geq |h_3|/p^2$ or $h_3 \geq |h_1|/p^2$.