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LETTER TO THE EDITOR

Gaussian smearing of spin weight functions in models of phase transitions

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Abstract. By smearing with a Gaussian distribution a family of single-spin weight functions is constructed which interpolates between an arbitrary single-spin distribution and a pure Gaussian. The observation of Baker and Bishop concerning the factorisability of the partition function of the double Gaussian model remains valid for all Gaussian-smeared models. The effects of smearing Gaussian and spherical weight functions are studied in further detail.

The statistical properties of a system with many degrees of freedom, say spins on lattice sites, depend not only on the nature of the point-to-point coupling, but also on the weight function which characterises the non-interacting single-spin distribution on each site. Since changes in the weight function can affect critical behaviour, it is instructive to study relationships between models with different weight functions. In this letter, we investigate a class of such relationships.

The weight function of the double-Gaussian model (Baker and Bishop 1982) interpolates between that of the spin-$\frac{1}{2}$ Ising model and that of a pure Gaussian model (Berlin and Kac 1952). This model has been studied recently, both to estimate corrections to scaling in Ising-like systems (Chen *et al* 1982) and to investigate the displacive to order–disorder crossover in structural transitions (Baker and Bishop 1982, Baker *et al* 1982). In particular, Baker and Bishop showed that the partition function of the double-Gaussian model with short-ranged interactions is the product of the partition function of a spin-$\frac{1}{2}$ Ising model with longer-ranged interactions and the partition function of a Gaussian model. Nickel (1981) pointed out that this decomposition allows one to define an analytic continuation of the model beyond the Gaussian and the Ising limits.

In this letter, we introduce a construction, 'Gaussian smearing', of a family of weight functions which interpolates between an *arbitrary* weight function and a Gaussian. We point out that the factorisability of the partition function noticed by Baker and Bishop in the double-Gaussian case holds equally for every such family, and use this result to discuss the crossover behaviour near the Gaussian limit. We also investigate two cases in a little more detail: (i) when the initial (unsmeared) weight function is a Gaussian; (ii) when the unsmeared spins obey a spherical constraint.

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Consider, to be specific, a system with scalar ($n=1$)-component continuous spins S with $-\infty<S<\infty$. If the initial weight function is $W_1(S)$, we define the Gaussian-smeared weight function by

$$W_y(\phi)=[2\pi(1-y)]^{-1/2}\int_{-\infty}^{\infty} \mathrm{d}S \exp\left(-\frac{(\phi-\sqrt{y}S)^2}{2(1-y)}\right) W_1(S). \tag{1}$$

With pairwise coupling K_{ij} between sites and an external field h, the partition function is taken to be

$$Z(\boldsymbol{K})=\int \prod_i \mathrm{d}\phi_i\, W_y(\phi_i) \exp\left(\tfrac{1}{2}\sum K_{ij}\phi_i\phi_j+h\sum \phi_i\right). \tag{2}$$

Since the kernel in (1) is designed to approach the delta function $\delta(\phi-S)$ as $y\to 1-$, the distribution $W_y(S)$ in general evolves smoothly into the original distribution $W_1(S)$ as y approaches 1. In general, if $W_1(S)$ is even and its second cumulant is finite and normalised to unity, the same is true of $W_y(\phi)$. The ratio of higher cumulant moments $\mu^{(2n)}(y)/\mu^{(2n)}(1)$ is then y^n for $n\geq 2$. As y varies between 0 and 1, $W_y(\phi)$ evolves from a Gaussian to $W_1(\phi)$. However, as pointed out by Nickel (1981) for the double-Gaussian model, and as discussed below for the general case, there is in general an analytic continuation to values of y *outside* this range.

On substituting (1) into (2), the ϕ integrations may be performed after shifting ϕ_i to

$$\phi_i'=\phi_i+\frac{\sqrt{y}}{1-y}\sum_j (M^{-1})_{ij}S_j+h\hat{M}^{-1}(0)\sum_i S_i. \tag{3}$$

The result can be written

$$Z(\boldsymbol{K})=Z_{\mathrm{G}}(\boldsymbol{M})Z(\boldsymbol{L}) \tag{4}$$

where the pure Gaussian factor is defined by

$$Z_{\mathrm{G}}(\boldsymbol{M})=(1-y)^{-N/2}(\det \boldsymbol{M})^{1/2}\exp(h^2\hat{M}^{-1}(0)) \tag{5}$$

while the new, non-trivial, factor is

$$Z(\boldsymbol{L})=\int \prod_i \mathrm{d}S\, W_1(S) \exp\left(\tfrac{1}{2}y\sum_{ij} L_{ij}S_iS_j+H\sum S_i\right). \tag{6}$$

If, as is usually appropriate to assume, the couplings K_{ij} are translationally invariant, the interaction matrices $\boldsymbol{M}=[M_{ij}]$ and $\boldsymbol{L}=[L_{ij}]$ are most conveniently defined in terms of their Fourier transforms. Thus one finds

$$\hat{M}(\boldsymbol{q})=(1-y)^{-1}-\hat{K}(\boldsymbol{q}) \tag{7}$$

$$\hat{L}^{-1}(\boldsymbol{q})=\hat{K}^{-1}(\boldsymbol{q})-(1-y) \tag{8}$$

where

$$\hat{K}(\boldsymbol{q})=\sum_j \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_{ij})K_{ij} \tag{9}$$

and $\hat{M}(\boldsymbol{q})$ and $\hat{L}(\boldsymbol{q})$ are defined similarly. The field H in (6) is given by

$$H=\sqrt{y}h/(1-\hat{K}(0)(1-y)). \tag{10}$$

If $y\neq 1$, the couplings yL_{ij} extend over all pairs i, j even if K_{ij} is non-zero only between nearest neighbour sites i, j. Suppose henceforth that the interactions K_{ij} are ferromagnetic so that $K_{ij} = K_{ji} \geq 0$ and that the lattice is bipartite. If $0 < y < 1$, the intersite couplings yL_{ij} are ferromagnetic and decay exponentially at large distances, with the range of interaction increasing as $y \to 0+$ (Baker and Bishop 1982). If $y < 0$, the couplings are antiferromagnetic, while if $y > 1$ there are couplings of both signs. For instance, in this latter case, on a simple cubic lattice yL_{ij} is ferromagnetic if site j can be reached from site i by taking an odd number of steps, and is antiferromagnetic if the number of steps is even. The ferromagnetic couplings are stronger.

Besides the relation between partition functions, other correspondences may be established: for instance the correlation functions are connected by

$$\chi_K(\boldsymbol{q}) \equiv \langle \phi_{\boldsymbol{q}} \phi_{-\boldsymbol{q}} \rangle_K = \frac{1-y}{1-(1-y)\hat{K}(\boldsymbol{q})} + \frac{y}{(1-(1-y)\hat{K}(\boldsymbol{q}))^2} \langle S_{\boldsymbol{q}} S_{-\boldsymbol{q}} \rangle_L \tag{11}$$

where

$$\phi_{\boldsymbol{q}} = N^{-1/2} \sum_i \exp(\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{R}_i) \phi_i \tag{12}$$

while $\langle \cdot \rangle_K$ denotes a thermal average with the weight function W_y and interactions K_{ij}, and $\langle \cdot \rangle_L$ denotes an average with weight function W_1 and interactions yL_{ij} (including yL_{ii}). If $y = 0$, the susceptibility $\chi_K(0)$ reduces to that of a Gaussian model with a transition at $\hat{K}(0) = 1$. If $y > 0$, there is, in general, a transition at a lower transition temperature, with distinct critical behaviour. The crossover near the multicritical point $y = 0$, $\hat{K}(0) = 1$ may be studied with the help of (11). For small y, we find the susceptibility

$$\chi_K(0) = (1 - \hat{K}(0))^{-1} + \tfrac{1}{2} y^2 \mu_4 L_{ii}^0 / (1 - \hat{K}(0))^2 \tag{13}$$

where μ_4 is the fourth cumulant moment of $W_1(S)$ and L_{ii}^0 is the $y = 0$ value of L_{ii}

$$L_{ii}^0 = \int \frac{\mathrm{d}\boldsymbol{q}}{1 - \hat{K}(\boldsymbol{q})} - 1$$

$$\to (A_d - 1) - B_d (1 - \hat{K}(0))^{(d-2)/2} \qquad \text{as } \hat{K}(0) \to 1, \tag{14}$$

where A_d is a d-dimensional Watson integral and B_d is a constant. Comparison with the conventional crossover form

$$\chi_K(0) \sim t^{-1} Y(g_y / t^{\phi}) \tag{15}$$

yields, for $d > 2$, the crossover exponent

$$\phi = (4 - d)/2 \tag{16}$$

and the scaling fields

$$g_y = y^2, \tag{17}$$

$$t = 1 - \hat{K}(0) + (1/e) y^2, \tag{18}$$

where the scaling axis slope e is given by

$$e^{-1} = -\tfrac{1}{2} \mu_4 (A_d - 1). \tag{19}$$

Let us now address some specific examples. If the original weight function W_1 is that of the spin-$\frac{1}{2}$ Ising model

$$W_1(S) = \tfrac{1}{2}[\delta(S-1) + \delta(S+1)] \tag{20}$$

we recover the results of Baker and Bishop for the double-Gaussian model. For that model, Nickel (1981) has pointed out that (5) and (6) define an analytic continuation of $Z(\boldsymbol{K})$ beyond $0 \leq y \leq 1$. However, the Gaussian partition function $Z_G(\boldsymbol{M})$ diverges once $\hat{M}(\boldsymbol{q})$ vanishes for any $\boldsymbol{q}$. Note that $\hat{L}(\boldsymbol{q})$ diverges at the same point.

These considerations on the continuation and on the divergence of $Z_G(\boldsymbol{M})$ apply also to the more general case considered here. For the ferromagnetic models on bipartite lattices that we are considering, $Z_G(\hat{M})$ converges in the region $-1 \leq \hat{K}(0)(1-y) \leq 1$. This is the unshaded region in figure 1. However, as we shall see below, the divergences of $Z_G(\boldsymbol{M})$ may sometimes be cancelled by $Z(\boldsymbol{L})$.

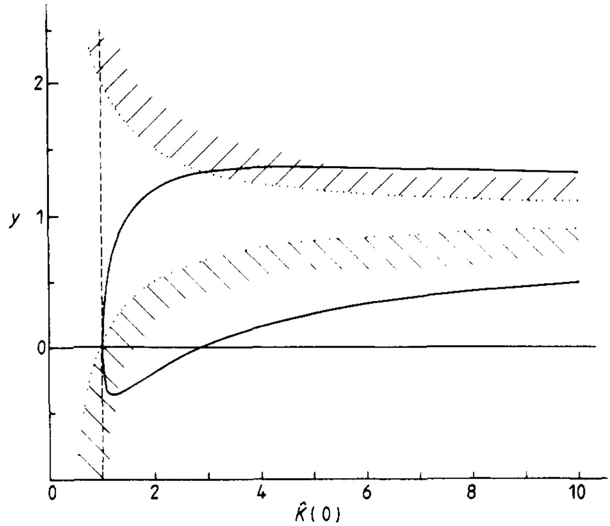

Figure 1. The typical phase diagram for Gaussian smeared models. As y varies from 0 to 1 the weight function evolves from a pure Gaussian to the unsmeared function W_1. The Gaussian partition function diverges along the dotted lines. Nevertheless the full partition function Zy for the special cases of the Gaussian and spherical models can be continued into the shaded region; the broken and full curves represent the critical lines for these two models.

Consider first the case when the original model is Gaussian, i.e.

$$W_1(S) = (2\pi)^{-1/2} \exp(-\tfrac{1}{2}S^2). \tag{21}$$

Then (1) gives $W_y(\phi) \equiv W_1(\phi)$ for all y. The critical line $\hat{K}(0) = 1$ (shown broken in figure 1) continues into the shaded regions and there is no other anomaly in the $(y, \hat{K}(0))$ plane. Although $Z_G(\boldsymbol{M})$ diverges at the boundary of the shaded region in figure 1, the product $Z(\boldsymbol{K}) = Z_G(\boldsymbol{M})Z(\boldsymbol{L})$ is well behaved. Similarly, there are cancellations between the two terms on the right-hand side of (5) so that $\chi(\boldsymbol{q})$ remains finite for $\hat{K}(0) < 1$.

Let us now incorporate a spherical constraint (Berlin and Kac 1952) by the replacement

$$\prod_i W_1(S_i) \Rightarrow \delta\left(\sum S_i^2 - N\right). \tag{22}$$

Now $Z(\boldsymbol{L})$ is the partition function of a spherical model with interactions yL_{ij}, and we have

$$\langle S_{\boldsymbol{q}} S_{-\boldsymbol{q}} \rangle = (z - y\hat{L}(\boldsymbol{q}))^{-1} \tag{23}$$

where in the disordered phase z is determined by the usual mean spherical constraint

$$\int \mathrm{d}\boldsymbol{q}\, \langle S_{\boldsymbol{q}} S_{-\boldsymbol{q}} \rangle = 1 \tag{24}$$

which can be rewritten as

$$y \int \frac{\mathrm{d}\boldsymbol{q}}{z - [y + z(1-y)]\hat{K}(\boldsymbol{q})} = y + (1-y)(z-1). \tag{25}$$

At criticality, one has $z = y\hat{L}(0)$, and the spherical condition determines the equation of the critical line as

$$\hat{K}_c(0) = \frac{2(1-y)A_d + 2y - 1 \pm [(2y-1)^2 + 4A_d y(1-y)]^{1/2}}{2(1-y)^2(A_d - 1)} \tag{26}$$

where

$$A_d = \int \frac{\hat{K}(0)\, \mathrm{d}\boldsymbol{q}}{\hat{K}(0) - \hat{K}(\boldsymbol{q})}. \tag{27}$$

If K_{ij} is non-zero for nearest neighbour pairs (i, j) only, A_d is Watson's integral (with $A_d \approx 1.5164$ for a simple cubic lattice).

From (11) we find the susceptibility is

$$\chi_K(0) = [z(1-y) + y]/\{z - [y + z(1-y)]\hat{K}(0)\}. \tag{28}$$

Evidently $\chi_K(0)$ diverges along the critical line with Gaussian exponents if $y = 0$ and spherical model exponents elsewhere.

As with the Gaussian model, the critical line continues smoothly into the shaded regions. $Z_G(\boldsymbol{M})$ diverges along the boundary of the shaded region but the product $Z_G(\boldsymbol{M})Z(\boldsymbol{L})$ is well behaved, suggesting that formulae such as (28) may provide analytical continuations into the shaded region. Note that the continuations of the critical line bend over and approach $y \to 1$ as $\hat{K}(0) \to \infty$, implying the loss of order at low temperatures (re-entrant behaviour).

However, the absence of anomalies along the loci $\hat{K}(0)(1-y) = \pm 1$ for the Gaussian and spherical models is probably peculiar to these models; for models with weight functions which decay more rapidly than Gaussian, we expect both $Z_G(\boldsymbol{M})$ and $Z(\boldsymbol{K})$ to diverge along the boundaries of the shaded regions. For example suppose

$$W_1(S) \sim \exp(-c|S|^\alpha) \qquad \text{as } |S| \to \infty \tag{29}$$

where c is a positive constant and $\alpha > 2$. Then (1) gives

$$W_y(\phi) \sim \exp[-\phi^2/2(1-y) - c'\phi^{\alpha/(\alpha-1)}] \tag{30}$$

as $|\phi| \to \infty$. Here c' depends on c, α and y, but the important point is that $\phi^{\alpha/(\alpha-1)}$ becomes negligible in comparison with ϕ^2 as $\phi \to \infty$. Thus the large ϕ contribution to the integrals in (2) is essentially the same as from the Gaussian factor, and so both $Z_G(\boldsymbol{M})$ and $Z(\boldsymbol{K})$ diverge along the boundaries of the shaded region in figure 1. An interesting unanswered question concerns the nature of the singularity in $\langle S_{\boldsymbol{q}} S_{-\boldsymbol{q}} \rangle_L$ at the intersection of the critical curve and the boundary of the upper shaded region for models of the type (29).

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