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Information geometry of finite Ising models☆

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Abstract

A model in statistical mechanics, characterised by a Gibbs measure, inherits a natural parameter-space geometry through an embedding into the space of square-integrable functions. This geometric structure reflects the underlying physics of the model in various ways. Here, we study the associated geometry and curvature for finite one- and two-dimensional Ising models as the lattice size N is varied. We show that there are temperature T and magnetic field h dependent critical values for the system size $N^*(T, h)$ where the curvature varies rapidly and undergoes a change of sign. Such finite volume geometric transitions are necessarily continuous. By comparison with known indicators, we demonstrate that the criterion $N \gg N^*$ provides a consistent constraint that lattice systems are qualitatively in their thermodynamic regime.

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1. Introduction

In the area of parametric statistics, it has long been known that a useful and illuminating approach is to view statistical models as characterised by differentiable manifolds $\mathfrak{M}$, equipped with a metric structure. Of particular interest in statistical inference is the notion of statistical divergence that measures the separation of two probability distributions, which

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is applied to study affinities amongst a given set of populations [1–4]. In particular, it was observed by Rao [5] that, for a parametric family of probability distributions, this divergence can be measured by the geodesic distance determined from the Fisher–Rao information metric [6,7].

A natural arena in which to apply the tools of information geometry is statistical mechanics, wherein $\mathfrak{M}$ is coordinatised by the external parameters of the system, such as temperature, pressure, external fields, and so on. In recent years a number of different models have been investigated within this formalism [8–12] (see [13] for a comprehensive list of references). The geometric structure with which the manifold $\mathfrak{M}$ is endowed leads to certain local invariants, one of the most important being the Ricci scalar curvature $\mathcal{R}$, and in the context of statistical mechanics one may enquire into the physical characteristics of the system which are encoded therein. In the thermodynamic limit, this question has been addressed in a number of models, with the conclusion that, in those cases exhibiting second-order phase transitions, the curvature of the thermodynamic parameter space $\mathfrak{M}$ diverges at the critical point. Moreover, the scaling behaviour of the curvature in the vicinity of the critical point is identical to that of the correlation volume. In other words, there is a scaling relation [11,13]

$$\mathcal{R} \sim \xi^d, \tag{1}$$

where ξ is the correlation length and d denotes the number of spatial dimensions of the model.

The scaling behaviour of the curvature provides a satisfying picture of how certain universal features of the near-critical regime are encoded in the Fisher–Rao geometry of $\mathfrak{M}$. However, it is also apparent that such a relation cannot be extended away from the regime of universality near second-order critical points. The correlation length is determined by the two-point functions of the theory while, as we shall discuss in more detail below, the curvature also receives contributions from higher order correlations. This begs the question of how, as we move away from the critical points in $\mathfrak{M}$, the deviation between $\mathcal{R}$ and ξ^d should be interpreted in physical terms. In particular, it is clear from this line of thought that the physical information encoded in geometric invariants like the scalar curvature must go well beyond universal characteristics such as (1).

Understanding the physical content of nonuniversal corrections to the curvature is a nontrivial problem in general, and need not have a generic answer. As a step towards this goal, we will study a related problem, namely the manner in which finite volume effects manifest themselves within information geometry. At first sight, one might anticipate from (1) that the curvature will exhibit finite-size scaling in systems that possess second-order critical points in the thermodynamic limit, and thus can act as a 'precursor' (cf. [14,15]) for second-order phase transitions. However, while this is undoubtedly the case, we have observed a rather more dramatic characteristic of the curvature which is an enhanced sensitivity to changes in the system size precisely in the regime where the thermodynamic character is lost through large finite size effects.

The problem of characterising the deviation from thermodynamic behaviour in finite lattice systems has recently been stimulated by advances in the condensed matter physics of mesoscopic-scale substances. Several investigations have focussed in particular on the existence of metastable phases in small lattice models [16,17]. Consequently, an important physical question to address in this context is when can a statistical mechanical system be regarded as ‘large’, or in its thermodynamic regime? Recent studies have shown [18] that there is often a quite precise critical size, that we will call N^*, above which the system is to a reasonable approximation ‘thermodynamic’. When the size drops below N^* the system often behaves in a qualitatively different way. Naturally, one may anticipate that such effects will be enhanced near second-order critical points where the correlation length grows large.

We will provide evidence that the information geometry is highly sensitive to these transitions, and that the curvature itself is a useful observable for indicating the transition of the system away from its thermodynamic regime. Specifically, we will consider lattice spin systems for which the system size N is conveniently measured by the number of lattice sites. We then find that the curvature $\mathcal{R}(N)$, as a function of N, exhibits a drastic change in its behaviour near the critical size N^*. For models with a parameter space of dimension 2 or higher, the most pronounced feature is that, although $\mathcal{R}$ is strictly positive in the thermodynamic regime, as one lowers the system size through N^*, the curvature undergoes a large gradient deviating rapidly from its thermodynamic value and passes through 0. We will refer to the lowest value of N for which the curvature remains positive as N_+. The critical value N_+ is parameter dependent and consequently, for fixed N, there is a boundary in $\mathfrak{M}$ where the curvature vanishes. Our main conclusion is that $N_+ \sim N^*$ and thus we can roughly interpret this boundary as separating thermodynamic (positive curvature) and nonthermodynamic (negative curvature) domains. We will provide evidence for this association by comparing the behaviour of the curvature with a more standard indicator of finite size corrections, namely the Binder [19] cumulant. These two measures indeed provide similar estimates for N^*.

The paper is organised as follows. We first recall how statistical models are endowed with a natural geometry in Section 2. Then, to illustrate the behaviour of the curvature in the thermodynamic regime, and also to motivate the association with finite size indicators, we discuss in Section 3 the simplified system of a one-dimensional parameter space. We then turn to the Ising model in an external field as our primary model of interest, which possesses a two-dimensional parameter space. After introducing the thermodynamic geometry in Section 4, we turn in Sections 5 and 6 to study the finite volume behaviour of the curvature, exhibiting its utility as an indicator of significant deviations from the thermodynamic regime. The one-dimensional Ising model is analysed in Section 5, while the two-dimensional Ising model is studied using Monte Carlo techniques in Section 6. We finish with some concluding remarks in Section 7.

2. Information geometry in statistical mechanics

Before turning to specific examples, we first review the manner in which models in statistical mechanics may be endowed with a natural geometric structure on the space of external parameters.

To begin, we recall that the state of a system immersed in a large heat bath with a fixed temperature T is given, in thermal equilibrium, by the Gibbs measure

$$p(x|\theta) = \exp\left(-\sum_{i=1}^{r}\theta^i H_i(x) - \ln Z(\theta)\right), \tag{2}$$

where the functions $H_i(x)$ on the phase space reflect terms in the Hamiltonian, $Z(\theta)$ is the partition function, and $\{\theta^i\}$ are thermodynamic variables which may include inverse temperature, pressure, magnetic field, chemical potential, and so on. We assume that the density function $p(x|\theta)$ is twice differentiable in the parameter θ. We note that the Gibbs measure should in fact be written $p(H(x)|\theta)$ because from a probabilistic point of view it is a function of energy. Nevertheless, we use a simplified notation which should not cause any confusion.

Given such a density function, we can map this to an element in the Hilbert space $\mathcal{H}$ of square-integrable functions [7] by the prescription

$$p(x|\theta) \mapsto \psi_\theta(x) = \sqrt{p(x|\theta)}. \tag{3}$$

Then, because of the normalisation condition for $p(x|\theta)$, the element $\psi_\theta(x) \in \mathcal{H}$ represents, for each fixed value of $\{\theta^i\}$, a point on the positive orthant of the unit sphere $\mathcal{S}$ in the Hilbert space. By continuously varying the values of $\{\theta^i\}$, this point moves inside an r-dimensional subspace of $\mathcal{S}$. This subspace is the thermodynamic parameter space, or, for the above Gibbs measure, the maximum entropy manifold $\mathfrak{M}$, and the metric on $\mathfrak{M}$ induced by the underlying spherical geometry of $\mathcal{S}$ is called the Fisher–Rao metric [5,20]. In particular, if we choose the parametrisation as given in (2) and write $\partial_i = \partial/\partial\theta^i$, then this metric takes the simple form

$$G_{ij} = 4\int \partial_i\psi_\theta(x)\partial_j\psi_\theta(x)\,\mathrm{d}x = \partial_i\partial_j \ln Z(\theta) \tag{4}$$

from which the curvature can be computed via standard prescriptions in Riemannian geometry. Note that here and in what follows we shall implicitly work with the metric density, obtained by dividing the free energy $\ln Z$ by the system size N, which is well-defined in the thermodynamic limit $N \to \infty$.

3. Extrinsic curvature of one-parameter statistical models

In order to gain some insight into which aspects of the physics are encoded in the geometry, both in the thermodynamic regime and in finite systems, it proves instructive to study a one-parameter family of thermal states ψ_β parameterised by the inverse temperature variable $\beta = 1/kT$, and analyse the role of the only natural invariant, the extrinsic curvature.

More precisely, the one-parameter family of canonical thermal states ψ_β is determined by the solution of the differential equation

$$\frac{\partial\psi_\beta}{\partial\beta} = -\frac{1}{2}\left(H(x) - \langle H\rangle\right)\psi_\beta, \tag{5}$$

where $\langle H\rangle$ is the expectation of the Hamiltonian $H(x)$ in the thermal equilibrium state ψ_β. The specification of the unique initial condition ψ_0 at infinite temperature then determines the manifold $\mathfrak{M}$, which in this case is a curve parameterised by β [21]. It follows from (5) that the extrinsic curvature K_ψ of $\mathfrak{M}$ is given by

$$K_\psi(\beta) = \frac{\langle\tilde{H}^4\rangle}{\langle\tilde{H}^2\rangle^2} - \frac{\langle\tilde{H}^3\rangle^2}{\langle\tilde{H}^2\rangle^3} - 1, \tag{6}$$

where

$$\langle \tilde{H}^n \rangle = \int \psi_\beta^2 \,(H(x) - \langle H \rangle)^n \; \mathrm{d}x \tag{7}$$

denotes the nth central moment of the Hamiltonian $H(x)$. When the dimension of the Hilbert space $\mathcal{H}$ is infinite, the statistical model may exhibit a phase transition at a critical point $\beta_\mathrm{c} = 1/kT_\mathrm{c}$, where the trajectory ψ_β on the unit sphere $\mathcal{S}$ proliferates into L distinct curves, where L is the multiplicity of the ground state. Physically, the ambiguity reflects the various coexisting phases allowed at the critical point. In particular, if the transition is of second-order, the curvature is singular at β_c. It follows from the expression (6) that the scaling behaviour of K_ψ around β_c is given by

$$K_\psi \sim \left| \frac{\beta_\mathrm{c} - \beta}{\beta} \right|^{-\kappa}, \tag{8}$$

where $\kappa = 2 - \alpha$ in terms of the conventional critical exponents. The standard relation $2 - \alpha = d\nu$ [22] then demonstrates that the curvature indeed scales like the correlation volume [9,11,13,23], as stated in the previous section.

As discussed above, we also expect the information geometry to encode nonuniversal features of the system. This is motivated here by the observation that the curvature (6) depends on third- and fourth-order cumulants, while the correlation length is known to be a second-order quantity. We then anticipate deviations to arise away from the critical regime, and through finite size corrections. Specifically, we see that K_ψ can be written as

$$K_\psi = 2 - B_\psi - S_\psi, \tag{9}$$

where $B_\psi = 3 - \langle \tilde{H}^4 \rangle / \langle \tilde{H}^2 \rangle^2$ is the Binder [19] cumulant determined by the kurtosis of the distribution, while $S_\psi = \langle \tilde{H}^3 \rangle^2 / \langle \tilde{H}^2 \rangle^3$ is the skewness. Note that B_ψ has long been used as a means of extracting first-order critical points from finite-size scaling. Hence this decomposition makes it clear that K_ψ must be sensitive to changes in the system size.

We will argue that such an interpretation is also possible for the intrinsic curvature of two-dimensional parameter-space manifolds, and we consider in particular the Ising model in an external field. Moreover, we will find that the intrinsic curvature exhibits a very characteristic dependence on the size as the system leaves its thermodynamic regime.

4. Ising models: geometry in the thermodynamic limit

Before turning to the analysis of finite size effects on the Ising model curvature, we first discuss aspects of the geometry of $\mathfrak{M}$ in the thermodynamic limit. For this purpose, we will consider the two-dimensional Ising model, and although much of what we discuss in this section is known, we will provide an information-geometric characterisation of phase transitions that is somewhat distinct from that already extant in the literature.

For the Ising spin model, we take $r = 2$ in equation (2), where $H_1(x)$ is the spin–spin interaction energy, $H_2(x)$ is the spin–field interaction energy, and $(\theta^1, \theta^2) = (\beta, h)$, where $\beta = 1/kT$. Thus, $Z(\theta)$ is a function of two variables, namely temperature and external magnetic field. In such cases where $\mathfrak{M}$ is two-dimensional, the intrinsic scalar curvature

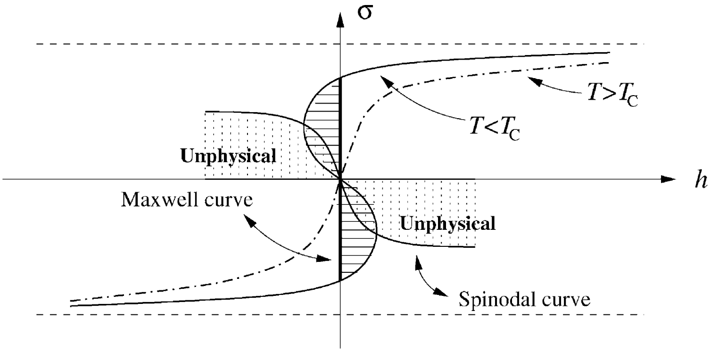

Fig. 1. A schematic illustration of the equation of state for the Ising model. The scalar curvature on the parameter space diverges along the spinodal boundary which envelopes the unphysical region. Thus, one can take the viewpoint that the curvature in some sense 'prevents' entrance to the unphysical domain.

assumes a simple form

$$\mathcal{R} = -\frac{1}{2G^2}\begin{vmatrix} \partial_1^2 \ln Z & \partial_1\partial_2 \ln Z & \partial_2^2 \ln Z \\ \partial_1^3 \ln Z & \partial_1^2\partial_2 \ln Z & \partial_1\partial_2^2 \ln Z \\ \partial_1^2\partial_2 \ln Z & \partial_1\partial_2^2 \ln Z & \partial_2^3 \ln Z \end{vmatrix}, \tag{10}$$

where $G = \det(G_{ij})$.

With this relation at hand, we are now in a position to study the geometric viewpoint on the equilibrium state of the system as one lowers the temperature through the phase transition at $T = T_c$. Firstly, we recall that the standard analysis (see e.g. [24]) for the Ising model in two or higher dimensions shows that the equation of state for the order parameter, i.e., the magnetisation per spin $\sigma(h)$, has the behaviour illustrated in Fig. 1. At temperatures below the Curie point T_c, the equation of state exhibits an essentially unphysical behaviour, namely the order parameter σ decreases in increasing external field h. The conventional argument is to apply Maxwell's equal area rule to follow through the transition as indicated in Fig. 1. Note, however, that not all the region beyond the Maxwell boundary is entirely unphysical, because in some parts the order parameter σ increases in decreasing h. The unphysical region, on the other hand, is surrounded by the spinodal curve along which $\partial\sigma/\partial h = \infty$, which also contains the transition point where $h = 0$.

These features are reflected in the geometry of the parameter space $\mathfrak{M}$ in the following way. For the Ising model in two dimensions, the scalar curvature $\mathcal{R}$ diverges at the transition point, as well as along the entire spinodal curve. The scaling of the curvature in this regime is again determined by the correlation volume as demonstrated in [11]. The divergence of the curvature on the spinodal boundary provides a 'geometric exclusion' from the unphysical domain. The presence of this divergence may be understood by taking a Legendre transform of the Fisher–Rao metric, which is given by the Hessian matrix of the entropy

$$g_{ab} = \partial_a\partial_b S \tag{11}$$

with respect to the extensive variables of the system. This metric, called the entropy derivative metric, first introduced by Rao, has also been applied to study statistical mechanical systems by Ruppeiner [13]. One observes that the nondegeneracy condition for this metric is precisely the concavity condition for the entropy, $\det(g_{ab}) > 0$, and thus its breakdown, where the curvature diverges, does indeed signal either a phase transition point or the presence of a spinodal boundary.

At a qualitative level, the physical behaviour of the system on traversing the spinodal boundary is also encoded in the connectedness of the surface $\mathfrak{M}$ on the unit sphere $\mathcal{S}$. In the absence of a phase transition, $\mathfrak{M}$ is a smooth manifold. However, if a transition exists, then below the transition temperature, i.e., 'beyond' the spinodal curve where the curvature diverges, the maximum entropy surface $\mathfrak{M}$ proliferates into two surfaces, associated with the two distinct ground states (all spins up or all spins down). More precisely, if we start with a pure thermal state $|\psi_\theta\rangle$ at high temperature, pure in the sense that for a fixed θ it is a uniquely defined state in the real Hilbert space $\mathcal{H}$, then by reducing the temperature adiabatically, this pure state 'evolves' into a mixed state $\sum_j \rho_j|\sigma_j\rangle\langle\sigma_j|$ where ρ_j determines the probability that the system magnetisation is σ_j. By a suitable measurement to determine the magnetisation of the system, this mixed state reduces to a pure state $|\sigma_k\rangle$, assuming that the measurement outcome is σ_k. This situation is illustrated in Fig. 2. Note that the 'evolution' described here only determines how an equilibrium state changes from one temperature to another, and there is no real finite-time dynamics involved.

In a more generic scenario of a phase transition for spin systems, we see that, in the absence of a symmetry breaking field, the pure state characterising the equilibrium configuration turns into a mixed state, reflecting the multiplicity of the ground state, through a geometric singularity. This, in a nutshell, is the information-geometric picture associated with symmetry breaking phase transitions. Although the calculations involved in such an analysis are rather involved, the two-dimensional Ising model at vanishing external field

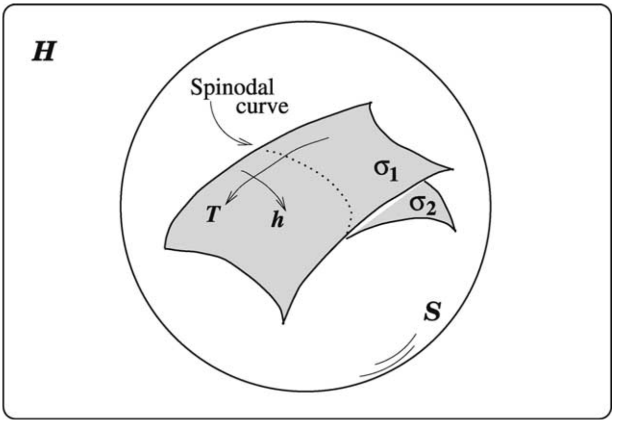

Fig. 2. A schematic representation of the maximum entropy surface for the two-dimensional Ising model on the unit sphere $\mathcal{S}$ in the Hilbert space $\mathcal{H}$. At high temperatures, the surface is uniquely defined, while at low temperatures, the surface is multi-valued, and can be labelled by the degeneracies of the ground state. Without further information, such as the presence of symmetry breaking field, we cannot identify which one of the surfaces the equilibrium state would reach beyond the spinodal curve.

provides a useful testing ground due to the existence of the exact Onsager solution, from which the curvature may be computed explicitly.

5. Ising chain: finite-size effects

The discussion of the preceding section illustrates how the information geometry captures certain universal features of the system in the thermodynamic limit. We now turn to consider the impact on the geometry of a reduction in the number of lattice points in the system.

For the two-dimensional parameter manifold $\mathfrak{M}$, the statistical geometry turns out to be quite sensitive to variations in the system size. However, what is perhaps more surprising is that the scalar curvature responds to variations in system size in a manner which provides a precise geometric characterisation of the transition between 'small' (nonthermodynamic) and 'large' (thermodynamic) systems. In particular, for the Ising model, as the number of lattice points N is reduced the scalar curvature remains close to its thermodynamic value, which is positive throughout the parameter space, until we reach a parameter-dependent critical value $N^*(\theta)$ where deviations first appear. The remarkable feature is that this transition is rapidly followed by a large gradient in the curvature accompanied by a change of sign. The critical value N_+ beyond which the curvature becomes negative is numerically close to N^*, particularly near the trivial critical point at $T = 0$. The association $N^* \sim N_+$ is tested and confirmed by comparing N_+ with the value of N^* determined from a more standard indicator of finite size effects, specifically the magnetic Binder cumulant. Thus, we are able to interpret the critical values $N_+(\theta)$ as a useful characterisation of the transition regime from 'small' to 'large' systems. We also find that for a given N, there is a submanifold of the parameter space $\mathfrak{M}$ on which the curvature vanishes, separating two domains of positive and negative curvature. We can then interpret the positive (respectively, negative) curvature domain as the parameter region in which the qualitative behaviour of the system is roughly thermodynamic (respectively, nonthermodynamic).

To illustrate these features, we now focus on the Ising model, as a convenient tractable example. We recall that the parameter space is two-dimensional with, as in Section 4, $H_1(x)$ the spin–spin interaction energy, and $H_2(x)$ the spin–field interaction energy. The Ricci scalar curvature (10) can be rewritten in the form

$$\mathcal{R} = -\frac{1}{2}\frac{\sum c_{ijlmpq}\langle\tilde{H}_i\tilde{H}_j\rangle\langle\tilde{H}_1\tilde{H}_l\tilde{H}_m\rangle\langle\tilde{H}_2\tilde{H}_p\tilde{H}_q\rangle}{(\sum \epsilon_{rs}\langle\tilde{H}_1\tilde{H}_r\rangle\langle\tilde{H}_2\tilde{H}_s\rangle)^2} \tag{12}$$

with appropriate coefficients ϵ_{rs}, $c_{ijlmpq} = 0, \pm 1$. This representation suggests its interpretation as a natural two-dimensional generalisation of the 'skewness' of the distribution. The intrinsic curvature thus depends only on second- and third-order cumulants, in contrast to the extrinsic curvature in (6). Nonetheless, we will show that $\mathcal{R}$ also acts as a clear indicator of finite size effects.

We consider first the one-dimensional Ising chain in an external field. The Hamiltonian for the system can now be written explicitly as

$$-\beta H = \beta\sum_{i=1}^{N} s_i s_{i+1} + h\sum_{i=1}^{N} s_i, \tag{13}$$

where $\{s_i = \pm 1\}$ are the spin variables, and $\beta = 1/kT$. The components of the Fisher–Rao metric are obtained by differentiating $N^{-1}\ \ln\ Z(\beta, h)$

$$G_{ij} = \frac{1}{N}\partial_i\partial_j\{N\beta + \ln[(\cosh h + \eta)^N + (\cosh h - \eta)^N]\}, \tag{14}$$

where $\eta = \sqrt{\sinh^2 h + \mathrm{e}^{-4\beta}}$. If we compute the metric in the thermodynamic limit $N \to \infty$, then the resulting expression simplifies, and we obtain the thermodynamic curvature, given by

$$\mathcal{R} = 1 + \eta^{-1}\cosh h, \tag{15}$$

which is always positive [9,11]. However, for finite N we observe that the curvature is no longer strictly positive and, as noted in [23], for a given point on the parameter space the curvature $\mathcal{R}$ can decrease and eventually becomes negative as N is reduced. Indeed, the transition to large negative values over a small range in N is quite marked. Some transition curves for $N_+(T)$ as a function of T (setting $h = 0.2$) are shown in Fig. 3.

This behaviour motivates the proposal that the rapid transition of the curvature as N passes through N_+ may provide a convenient indicator of the departure of the system away from its thermodynamic regime, i.e., when the system changes from being large to small. To test this proposition, a natural quantity to use for comparison is the magnetic Binder cumulant $B_h = 3 - \langle\tilde{H}_2^4\rangle/\langle\tilde{H}_2^2\rangle^2$. The N-dependence of this observable is shown in Fig. 4. Finite N corrections again become apparent near the critical point. One sees that the size $N^*(T)$, at which deviations from the thermodynamic limit first become apparent quite closely matches that of the curvature $N_+(T)$ shown in Fig. 3. Indeed, the correspondence is rather better

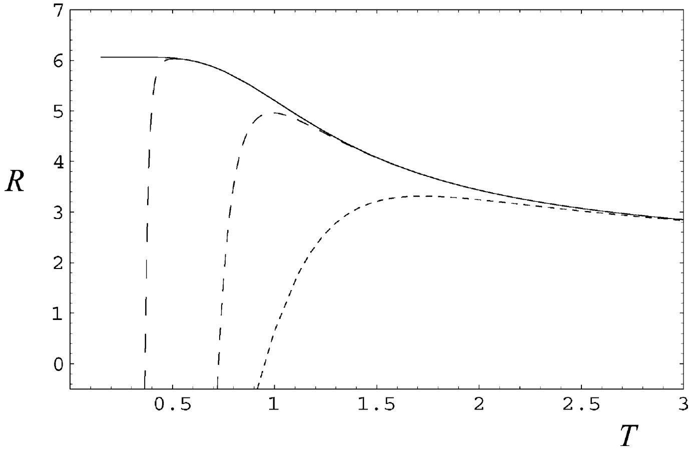

Fig. 3. A plot of thermodynamic curvature $\mathcal{R}(T)$ for the one-dimensional Ising model, with $h = 0.2$, for $N = 10, 20$ and 50. The solid line is the curvature in the thermodynamic limit, and deviations from this behaviour are soon followed by the rapid transition of the curvature to large negative values. The curvature vanishes when $N_+(T \sim 0.45) = 50$, $N_+(T \sim 0.7) = 20$ and $N_+(T \sim 1) = 10$. The conjectured association $N^* \sim N_+$ thus holds increasingly well near the critical point.

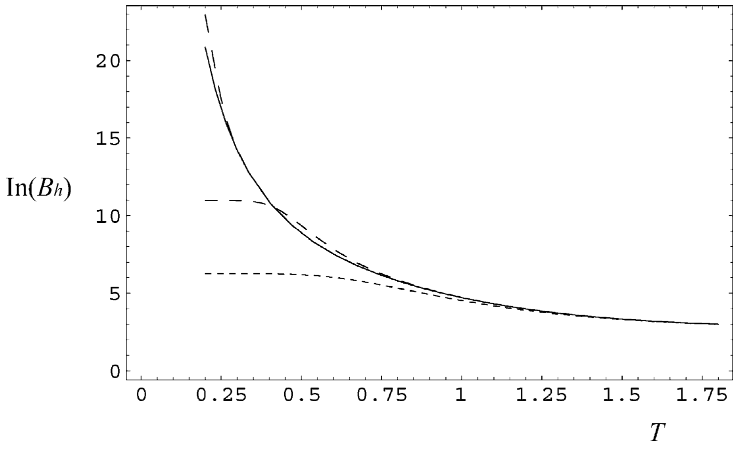

Fig. 4. A logarithmic plot of the Binder cumulant for the one-dimensional Ising model, with $h = 0.2$, as a function of T. The solid line represents the thermodynamic limit, and finite size deviations first occur at $N^*(T \sim 0.35) = 50$, $N^*(T \sim 0.8) = 20$ and $N^*(T \sim 1.2) = 10$. Note that the vertical axis has been shifted for convenience.

than might have been anticipated on comparing N_+ with the value of N at which the first signs of deviation from thermodynamic behaviour are apparent in Fig. 3.

This is the main result of this work and, as stated earlier, suggests that the information geometry, or more precisely the invariant curvature, is remarkably sensitive to the transition away from the thermodynamic regime as the system size is lowered.

We can now attempt to characterise the transition more precisely. In particular, these results suggest that there exists a connected region in parameter space where the curvature is negative, and a corresponding boundary where the curvature vanishes. This turns out to be the case, and the profile of the zero curvature subspace of $\mathfrak{M}$ can be obtained numerically. Results for several values of N are shown in Fig. 5.

The positivity of (15) implies that the negative curvature domain is 'metastable' in that it is present only for finite N. We find that as N increases it contracts to a region around the critical point. This is to be expected as it is only in this neighbourhood that finite size effects will be important when N becomes large. However, the presence of the negative curvature domain in the one-dimensional Ising model indicates that more generally it has little to do with precursors for genuine phase transitions in the thermodynamic limit.

Without attempting to delve into the specific physical features of the negative curvature domain, it is worth digressing slightly to note that the simplest geometric distinction with the positive curvature domain is the divergence of nearby geodesics. This suggests a possible characterisation through equations of state in the following way. Specifically, recall that a Taylor series expansion of the relative entropy $S(p|q) = \int p \ln(p/q)$ between two distributions p and q is given [25], to lowest order, by the Fisher–Rao line element

$$S(p(\theta)|p(\theta + \mathrm{d}\theta)) = \tfrac{1}{2} G_{ij}\, \mathrm{d}\theta^i\, \mathrm{d}\theta^j + \cdots . \tag{16}$$

Thus $\mathfrak{M}$ can be interpreted as a maximum entropy surface and consequently specific geodesics will correspond to equations of state for the system [10,25,26].

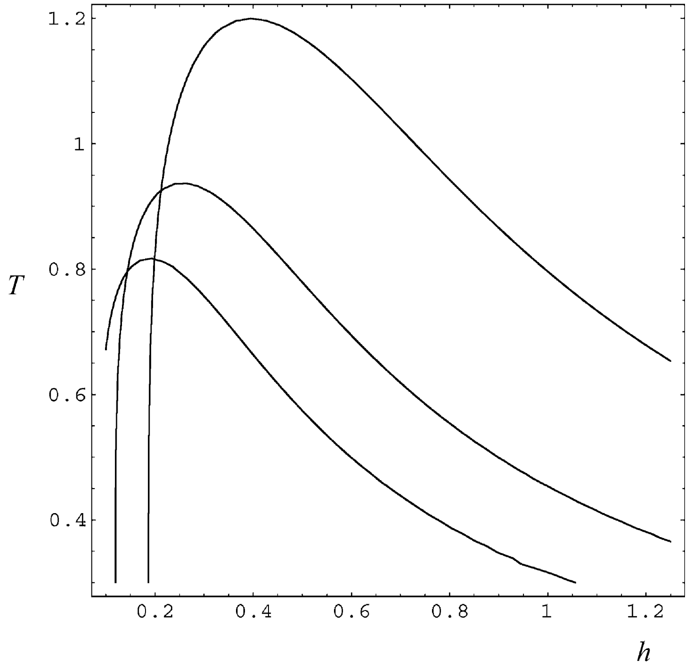

Fig. 5. We exhibit the negative curvature domains for the one-dimensional Ising chain. The curvature is negative in the low temperature phase, and vanishes along the curves shown, which correspond, from top to bottom, to $N = 8, 12$ and 16.

6. Two-dimensional Ising model: negative curvature domain

To explore the universality of these features, at least within the context of ferromagnetic spin models, we also studied the N-dependence of the curvature in the two-dimensional Ising model. The main new ingredient is the existence of a genuine phase transition in the thermodynamic limit. However, we observe that this has only a relatively minor effect on the behaviour of the curvature near $N^*(\theta)$ and on the characteristic positive and negative curvature domains in $\mathfrak{M}$. In particular, as N increases the 'metastable' negative curvature domain now contracts around the critical point at $T = T_c \sim 2.27$, rather than the critical point at $T = 0$ in the one-dimensional Ising model.

The Hamiltonian is now given by

$$-\beta H = \beta \sum_{i,j=1}^{N} (s_{ij}s_{i+1j} + s_{ij}s_{ij+1}) + h \sum_{i,j=1}^{N} s_{ij}, \tag{17}$$

parameterised again by the inverse temperature and magnetic field, except the spin variables $\{s_{ij}\}$ are now defined on a toroidal lattice. For the two-dimensional Ising model with an applied field, an analytical expression for $\ln Z$ is not available for generic N. However, Monte Carlo simulation is relatively straightforward in this case and it has in fact been

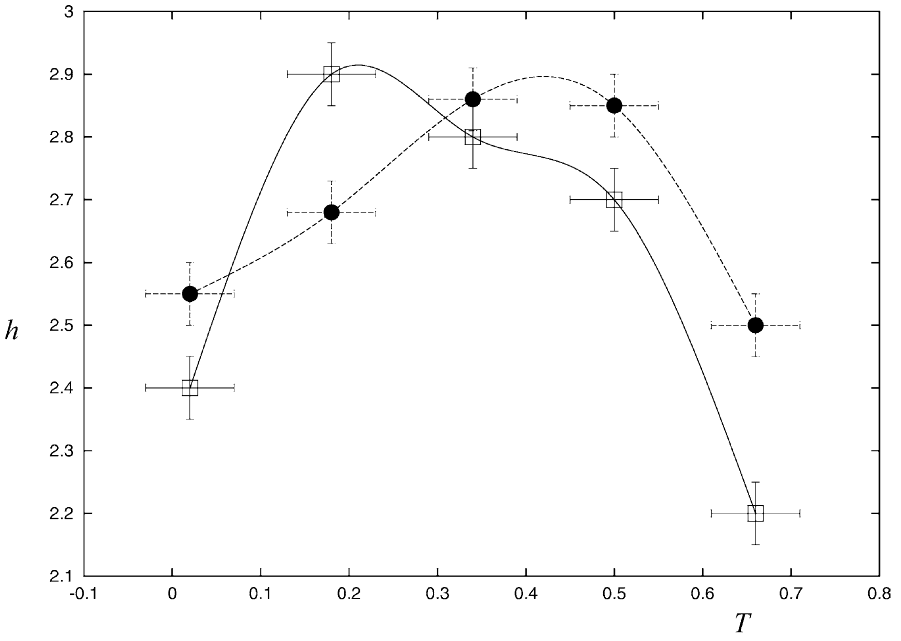

Fig. 6. An interpolation of the $\mathcal{R} = 0$ boundary for the two-dimensional Ising model. Results for the 8×8 and 16×16 lattices are represented by open squares and filled circles, respectively. The curvature is positive above (high h), and negative below (low h), the domain boundaries.

used before in the geometric context [27]. Indeed, as we note from (12), each entry in the determinant is a combination of central moments for terms in the Hamiltonian.

Because our primary aim is to provide evidence for the existence of a negative curvature domain in this system, we implemented a conventional Metropolis algorithm on small 8×8 and 16×16 lattices, in the parameter range where the negative curvature domain is expected to arise. The details of the simulations are as follows. The results for each individual measurement of $\mathcal{R}$ were combined from a set of 10^3 runs to obtain the quoted statistical errors, and there were 10^3 thermalisation steps prior to each sampling. The results were stable with respect to using hot or cold starts, and sequential or random site updates. This simple approach was sufficient for the qualitative issues we are concerned with here. However, it is likely that, for example, multicanonical methods as used in [16,17] may be more suitable for precise studies.

The results indeed indicate the presence of a negative curvature domain for finite N, and the zero curvature boundary has been interpolated in Fig. 6. The relatively large errors are the result of significant cancellations between the third-order cumulants used to construct the curvature. An interesting point to note is that the boundary is fairly stable for the two system sizes, in contrast to the large shift observed in the one-dimensional case. This is clearly related to the presence of the critical point at ($T_c \sim 2.27, h = 0$) in the thermodynamic limit, around which the negative curvature domain shrinks. As in the one-dimensional model, the transition in the curvature from a value near its thermodynamic limit to negative values was very sharp on passing through $N_+(\theta)$. This is also reflected in the fact that the gradient of the curvature on the zero curvature boundary in Fig. 6 is large, and one does not need to move far from the boundary into the positive curvature domain for the curvature to approach its thermodynamic value. Thus the value of $N_+(\theta)$ determined in this manner again seems to provide a good indication of when the system leaves its thermodynamic regime.

7. Discussion

The use of geometric techniques in the wider context of parametric statistics has a long history [28], and this formalism has more recently been introduced as a useful tool in statistical mechanics. Currently, the application of this formalism is hindered by the lack of any detailed understanding of the physical interpretation of geometric invariants, such as the scalar curvature, away from the universal regime near second-order critical points.

In this paper, we have moved beyond the thermodynamic limit by studying the behaviour of the curvature in finite-size Ising models. The curvature was found to be sensitive to variation of the system size N, and most significantly was shown to undergo a rapid transition to a negative curvature regime as N was lowered through a critical value N_+. Comparison with a more standard finite size indicator—the Binder cumulant—allowed the interpretation of $N_+(\theta)$ as a useful characterisation of the transitional size for which the system changed from being in an essentially thermodynamic regime ($N > N_+$) to an essentially nonthermodynamic regime ($N < N_+$).

These results pose a number of open questions. Perhaps the most pertinent with regard to understanding the physical role of the curvature is whether there is a precise physical characterisation of what we might tentatively call the negative curvature 'phase'. Another issue is whether these features exist beyond the class of ferromagnetic spin models that we have studied here. In this regard, we conclude by noting that preliminary results for a similar analysis of the three-dimensional Ising model also clearly indicate the presence of a negative curvature region, although this domain in parameter space is somewhat smaller than that for the two-dimensional case above, for analogous lattice sizes.

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References

[1] P.C. Mahalanobis, On tests and measures of group divergence, J. Asiatic Soc. Bengal 26 (1930) 541.
[2] P.C. Mahalanobis, On the generalised distance in statistics, Proc. Nat. Inst. Sci. India 12 (1936) 49.
[3] A. Bhattacharyya, On a measure of divergence between two multinomial populations, Sankhyā 7 (1946) 401.
[4] C.R. Rao, The problem of classification and distance between two populations, Nature 159 (1947) 30.
[5] C.R. Rao, Information and the accuracy attainable in the estimation of statistical parameters, Bull. Calcutta Math. Soc. 37 (1945) 81.

[6] J. Burbea, C.R. Rao, Differential metrics in probability spaces, Prob. Math. Stat. 3 (1984) 241.
[7] J. Burbea, Informative geometry of probability spaces, Expo. Math. 4 (1986) 347.
[8] L. Diosi, G. Forgács, B. Lukács, H.L. Frisch, Metricization of thermodynamic-state space and the renormalization group, Phys. Rev. A 29 (1984) 3343.
[9] H. Janyszek, R. Mrugala, Riemannian geometry and the thermodynamics of model magnetic systems, Phys. Rev. A 39 (1989) 6515.
[10] H. Janyszek, Riemannian geometry and stability of thermodynamical equilibrium systems, J. Phys. A 23 (1990) 477.
[11] D. Brody, N. Rivier, Geometrical aspects of statistical mechanics, Phys. Rev. E 51 (1995) 1006.
[12] R.F. Streater, Classical and quantum info-manifolds, in: M. Ohya, N. Watanabe (Eds.), Quantum Information, Measurement and Computing, Kyoto, 2000.
[13] G. Ruppeiner, Riemannian geometry in thermodynamic fluctuation theory, Rev. Mod. Phys. 67 (1995) 605.
[14] D.H.E. Gross, E. Votyakov, Phase transitions in "Small" systems, Eur. Phys. J. B 15 (2000) 115.
[15] M. Promberger, M. Kastner, A. Hüller, Magnetic properties of finite systems: microcanonical finite size scaling, in: D.P. Landau, S.P. Lewis, H.B. Schuettler (Eds.), Computer Simulation Studies in Condensed Matter Physics XII, Springer, Berlin, 1999.
[16] J. Lee, M.A. Novotny, P.A. Rikvold, A method to study relaxation of metastable phases: macroscopic mean-field dynamics, Phys. Rev. E 52 (1995) 356.
[17] I. Shteto, J. Linares, F. Varret, Monte Carlo entropic sampling for the study of metastable states and relaxation paths, Phys. Rev. E 56 (1997) 5128.
[18] C.Y. Lin, S.N. Cho, C.G. Goedde, S. Lichter, When is a one-dimensional lattice small? Phys. Rev. Lett. 82 (1999) 259.
[19] K. Binder, Finite size scaling analysis of Ising model block distribution functions, Z. Phys. B 43 (1981) 119.
[20] D.C. Brody, L.P. Hughston, Statistical geometry in quantum mechanics, Proc. R. Soc. London A 454 (1998) 2445.
[21] D.C. Brody, L.P. Hughston, Geometrization of statistical mechanics, Proc. R. Soc. London A 455 (1999) 1683.
[22] H.E. Stanley, Introduction to Phase Transitions and Critical Phenomena, Oxford University Press, Oxford, 1971.
[23] D.C. Brody, A. Ritz, On the symmetry of real-space renormalisation, Nucl. Phys. B 522 (1998) 588.
[24] J.J. Binney, N.J. Dowrick, A.J. Fisher, M.E.J. Newman, The Theory of Critical Phenomena, Oxford University Press, Oxford, 1992.
[25] R.S. Ingarden, Information geometry in functional spaces of classical and quantum finite statistical systems, Int. J. Eng. Sci. 19 (1981) 1609.
[26] H. Janyszek, On the Riemannian metrical structure in the classical statistical equilibrium thermodynamics, Rep. Math. Phys. 24 (1986) 1.
[27] E.J. Brody, Applications of the kakutani metric to real space renormalization, Phys. Rev. Lett. 58 (1987) 179.
[28] R. Kass, The geometry of asymptotic inference, Stat. Sci. 4 (1989) 188.