Geometric Phase Transitions

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(September 11, 2018)

A model in statistical mechanics, characterised by the corresponding Gibbs measure, is a subset of the totality of probability distributions on the phase space. The shape of this subset, i.e., the geometry, then plays an important role in statistical analysis of the model. It is known that this subset has the structure of a manifold equipped with a Riemannian metric, given by the Fisher information matrix. Invariant quantities such as thermodynamic curvature have been studied extensively in the literature, although a satisfactory physical interpretation of the geometry has not hitherto been established. In this article, we investigate the thermodynamic curvature for one and two dimensional Ising models and report the existence of a geometric phase transition associated with a change in the signature of the curvature. This transition is of a continuous type, and exists for finite systems. The effect may be tested in principle by mesoscopic scale experiments.

PACS Numbers : 05.20.-y, 05.70.Fh, 02.40.Ky

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, equipped with the Fisher-Rao metric. Of particular interest in statistical inference is the notion of statistical divergence that measures how separated two probability distributions are, which is applied to study affinities amongst a given set of populations. It was discovered by Rao that this divergence can be measured by the geodesic distance determined from the Fisher information matrix [1]. Analogous studies have been made in statistical mechanics, and numerous models including those exhibiting phase transitions were investigated [2] (for a comprehensive list of references, see [3]). In particular, it was found that, for models exhibiting second order phase transitions, the curvature of the thermodynamic parameter space \( M \) diverges at the critical point, and that the scaling exponent of the curvature in the vicinity of the transition point is identical to that of the correlation volume [3]. Furthermore, for simple models such as the ideal gas, it has also been shown that the geodesic curves on \( M \) correspond to various equations of state for the system [4].

On the whole, most of the literature on the geometry of the thermodynamic parameter space has been devoted to analysing properties in the thermodynamic limit, owing to the interest in critical phenomena. In this paper, however, we investigate finite size (volume) effects in the thermodynamic curvature for one and two dimensional Ising models. In particular, it is shown that, for a finite number \( N \) of spins, the phase diagram is clearly divided into two phases, namely, the positive and negative curvature phases. Furthermore, this phase separation disappears as \( N \to \infty \). Because the size of the system is finite, the transition is continuous and is not accompanied by a singularity. Possible experimental realisations, based on the idea of generalised equations of state, are considered.

Before turning to the analysis of finite size effects on the thermodynamic curvature for the Ising models, we first introduce the basic ideas behind the geometric approach to statistical mechanics. For this purpose, we consider the van der Waals gas model for vapour liquid transitions, because this is a nontrivial model that has nonetheless been studied quite extensively.

In statistical mechanics, we begin by considering the probability distribution given by the Gibbs measure,

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

where \( H_i(x) \) are Hamiltonian functions on the phase space, \( Z(\theta) \) is the partition function, and \( \{\theta^i\} \) are thermodynamic variables which may include inverse temperature, pressure, magnetic field, chemical potential, and so on. This density can be mapped to an element in a Hilbert space [1] by the prescription \( p(x|\theta) \to \psi(x) = \sqrt{p(x|\theta)} \). Then, because of the normalisation condition for \( p(x|\theta) \), the square-integrable function \( \psi(x) \) represents, for each fixed value of \( \{\theta^i\} \), a point on the positive ‘octant’ of the unit sphere \( S \) in Hilbert space. By continuously changing the values of \( \{\theta^i\} \), this point clearly moves inside an \( r \)-dimensional subspace of \( S \). This subspace is the thermodynamic parameter space, or, for the above Gibbs measure, the maximum entropy manifold \( M \), and the metric on \( M \) induced by the underlying spherical geometry of \( S \) is called the Fisher-Rao metric. In particular, if we choose the parametrisation as given in [1] and write \( \partial_i = \partial/\partial \theta^i \), then this metric takes the simple form \( G_{ij} = \partial_i \partial_j \ln Z \), from which the curvature can be computed via standard prescriptions in Riemannian geometry.

Now suppose we consider the van der Waals model, where in equation (1) we take \( r = 2 \), \( H_1(x) \) the energy, \( H_2(x) \) the volume \( V \), and \( \{\theta^1, \theta^2\} = (1/kT, P/kT) \). Thus,
Considered later, the scalar curvature assumes a simple form along which increases in decreasing volume. The unphysical region, is entirely unphysical, because in some part the pressure that not all of the region inside the Maxwell boundary through the transition. This is sketched in Fig. 1. Note argument is to apply Maxwell’s equal area rule to follow decreases as the volume is reduced. The conventional argument can be further analysed by consideration of the spinodal boundary which envelopes the unphysical region. The scalar curvature on the parameter space diverges along the curve where the proliferation occurs. In the absence of any symmetry breaking field, the pure state characterising the equilibrium state turns into a mixed state through a geometric singularity, reflecting the multiplicity of the ground state. This is how the equilibrium theory for characterising symmetry breaking can be viewed in the geometric framework. Although the calculations involved here can be quite intricate, consideration of thermodynamic limit often leads to useful simplifications.

While the theory of critical phenomena is of great interest in the approach outlined above, owing to various advances in experimental condensed matter physics, there is also a growing interest in understanding the effect of a finite system size on thermodynamic quantities. This motivates us to study, in particular, such effects on the thermodynamic curvature. This will be analysed here by consideration of the Ising models in one and two dimensions. Let us first study the one-dimensional Ising chain. The Hamiltonian for the system is given by

\[-\beta \mathcal{H} = \beta \sum_{i=1}^{N} \sigma_i \sigma_{i+1} + h \sum_{i=1}^{N} \sigma_i,\]  

where \(\{\sigma_i = \pm 1\}\) are the spin variables, \(\beta = 1/(kT)\), and the two-dimensional manifold \(\mathcal{M}\) is parametrised by \((\theta^1, \theta^2) = (\beta, h)\). The components of the Fisher-Rao metric per spin are obtained by differentiating \(\ln Z(\beta, h)/N\):

\[R = -\frac{1}{2G^2} \begin{vmatrix} \frac{\partial^2 \ln Z}{\partial \theta^1 \partial \theta^2} & \frac{\partial^2 \ln Z}{\partial \theta^1 \partial \theta^2} & \frac{\partial^2 \ln Z}{\partial \theta^1 \partial \theta^2} \\ \frac{\partial^2 \ln Z}{\partial \theta^2 \partial \theta^2} & \frac{\partial^2 \ln Z}{\partial \theta^2 \partial \theta^2} & \frac{\partial^2 \ln Z}{\partial \theta^2 \partial \theta^2} \\ \frac{\partial^2 \ln Z}{\partial v \partial \theta^1} & \frac{\partial^2 \ln Z}{\partial v \partial \theta^2} & \frac{\partial^2 \ln Z}{\partial v \partial \theta^2} \end{vmatrix}, \]  

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

The phase space integral for the partition function is known to give rise to the cubic equation of state for the van der Waals model, which includes an essentially unphysical region in the parameter space where the pressure decreases as the volume is reduced. The conventional argument is to apply Maxwell’s equal area rule to follow through the transition. This is sketched in Fig. 1. Note that not all of the region inside the Maxwell boundary is entirely unphysical, because in some part the pressure increases in decreasing volume. The unphysical region, on the other hand, is surrounded by the spinodal curve along which \(\theta^2/\partial v = 0\), where \(v = v(\theta^1, \theta^2)\) is the mean volume determined by the equation of state. This curve also contains the transition point where \(\partial \theta^1/\partial v = 0\).

In the case of the van der Waals model, further physical arguments in fact rule out two of the unphysical roots for the equation of state, and we can single out one physical state \(|v_k\rangle\). However, in a generic scenario of a phase transition, in the absence of any symmetry breaking field, the pure state characterising the equilibrium state turns into a mixed state through a geometric singularity, reflecting the multiplicity of the ground state. This is how the equilibrium theory for characterising symmetry breaking can be viewed in the geometric framework. Although the calculations involved here can be quite intricate, consideration of thermodynamic limit often leads to useful simplifications.

**FIG. 2.** A schematic representation of the maximum entropy surface for the van der Waals model on the unit sphere \(S\) in Hilbert space. At high temperatures, the surface is uniquely defined, while at low temperatures, the surface is multi-valued, and can be labelled by the roots of the equation of state. Without further information, we cannot identify which one of the surfaces the equilibrium state would reach beyond the spinodal curve.
\[ G_{ij} = \frac{1}{N} \partial_i \partial_j \left\{ \ln \left[ (\cosh h + \eta)^N + (\cosh h - \eta)^N \right] \right\}, \quad (4) \]

where \( \eta = \sqrt{\sinh^2 h + e^{-4\beta}} \). Here, we set Boltzmann’s constant \( k = 1 \). If we compute the metric in the thermodynamic limit \( N \to \infty \), then the resulting expression simplifies, and we obtain the thermodynamic curvature \( \frac{2}{N} \), given by \( R = 1 + \eta^{-1} \cosh h \), which is always positive. However, if we consider finite size effects, we observe that the curvature is no longer strictly positive. In particular, it was noted in [6] that for a given point on parameter space, \( R \) could decrease and eventually become negative as \( N \) was reduced. Indeed, the transition to large negative values over a small range in \( N \) is quite marked as one may observe in Fig. 3 where we consider the point \( \{ T = 0.3, h = 0.4 \} \).

The result in Fig. 3 suggests the existence of a phase separation in terms of positive and negative curvatures. Indeed, because the components of the metric can be obtained explicitly for arbitrary finite \( N \), we can compute the curvature \( R \) as a function of \( N \) and then numerically extrapolate the phase boundary along which the curvature vanishes. The result is shown in Fig. 4 for several values of \( N \). Further numerical analysis shows that the parameter space is indeed separated into these two phases. Before seeking any physical consequences of this geometric phase separation, we would like to analyse the case of the two-dimensional Ising model, in order to indicate the universality of the phenomenon at least within the context of ferromagnetic spin models.

In the two-dimensional case, we also consider the Hamiltonian given in (3) parametrised by the inverse temperature and magnetic field, except the spin variables \( \{ \sigma_i \} \) 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 sufficiently large \( N \). However, a Monte Carlo simulation turns out to be quite effective in analysing problems of this kind.

In particular, if we return to the expression given in (3), we notice that each entry in the determinant is a combination of the products of central moments for terms in the Hamiltonian, and thus calculation of \( R \) is quite amenable to Monte Carlo analysis.

We simulated the Ising spins on \( 8 \times 8 \) and \( 16 \times 16 \) lattices, using a standard Metropolis algorithm, and the results were combined from a series of runs using alternately sequential and random site updates, and hot and cold starts. The values of \( R \) were computed for a range of values of \( (T, h) \), and the results clearly indicate the presence of a transition between positive and negative curvature regions. Numerical values for the curvature near this phase boundary, including statistical errors from a series of 10 runs with the differing initial conditions and update procedures mentioned above, are presented in Table I. The relatively large errors are a 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 shift observed in the 1D case. This is presumably related to the presence of the critical point at \( (T_c \sim 2.27, h = 0) \). Preliminary results for a similar analysis of the 3D Ising model also indicate a clear presence of a negative curvature region for low temperatures, although this region in parameter space is somewhat smaller than for the 2D case above.

In the foregoing analysis we have demonstrated the existence of positive and negative curvature phases for one and two dimensional Ising models. Whereas the discontinuities which are manifested in conventional phase transitions can only occur in the thermodynamic limit, these qualitative geometrical transitions occur even in the simplest finite-dimensional models.

The important issue we now address is whether there
is any physical or observational consequence of this transition. While the answer appears to be yes insofar as the curvature is at least indirectly measurable, a more intriguing consequence arises once we recall the fact that the deviation of a collection of nearby geodesic curves is conditioned by the Riemann curvature tensor. In particular, if we consider a set of nearby geodesics in a region of $\mathcal{M}$, then these geodesics will tend to deviate apart if $\text{sgn}(\mathcal{R}) < 0$, while the converse is true if $\text{sgn}(\mathcal{R}) > 0$. Furthermore, the geodesics on $\mathcal{M}$ can be viewed to play the role of generalised equations of state corresponding to different initial conditions. This can be seen from the fact that the leading term in the Taylor series expansion of the relative entropy is given by the infinitesimal line element $ds^2 = G_{ij}d\theta^i d\theta^j$. In other words, we have $S(p(\theta))p(\theta + d\theta) = \frac{1}{2} ds^2$ in the limit $d\theta \to 0$. Hence we see that a geodesic joining two nearby points on $\mathcal{M}$ corresponds to a trajectory that extremises the entropy, and thus has a natural parallel with an equation of state.

On the other hand, for any given point in $\mathcal{M}$ there are infinitely many geodesic curves that pass this point, each of which is subject to an initial condition, which may include the requirement of an adiabatic or isothermal change of the system. In this case, two nearby equations of state would deviate away if the sign of $\mathcal{R}$ is negative. Therefore, an experimental verification of the phase separation requires an extensive analysis of equations of state for various different processes. Given such data it may be possible to identify qualitatively different behaviours for the two phases.

In summary, we have shown the existence of phase separations in terms of the signature of the thermodynamic curvature for finite Ising spins in one and two dimensions. Owing to the fact that $\mathcal{R}$ is expressible in terms of correlation functions of order $\leq 6$ ($\leq 3$ in the present case), a Monte Carlo computation is straightforward, in contrast to the renormalisation group approach which generally requires knowledge of an infinite number of correlation functions. Therefore, it would be of interest also to analyse the curvature for lattice gauge theories in a finite volume. Finally, we have argued that geodesics on $\mathcal{M}$ generalise the notion of an equation of state, for arbitrary initial conditions, and thus experimental realisation may be obtained in principle by the analysis of equations of state for these systems at mesoscopic scales.

Another interesting open question in this regard is the direct physical interpretation of the curvature $\mathcal{R}$. We note that $\mathcal{R}$ is determined by the parallel transport of tangent vectors over $\mathcal{M}$. In particular, by following a closed contour $\mathcal{C}$ on $\mathcal{M}$, a tangent vector is rotated by an angle given by the integral of $\mathcal{R}$ over the area inside $\mathcal{C}$ (holonomy). In ordinary thermodynamics, Maxwell’s relations guarantee that any closed contour $\mathcal{C}$ is thermodynamically trivial, provided $\mathcal{C}$ does not surround a critical point or straddle the spinodal curve. Therefore, if there is a physical interpretation of tangent vectors over the maximum entropy surfaces, then the geometric notion of holonomy leads to a new thermodynamic property whereby a system does not return to its original state after going around a contour, a concept analogous to magnetic hysteresis.

DCB is supported by Particle Physics and Astronomy Research Council. The authors acknowledge N. Rivier for stimulating discussions.

1. Burbea, J., Expo. Math. 4, 347 (1986).
2. Diosi, L., Forgacs, G., Lukacs, B., and Frisch, H.L., Phys. Rev. A 29, 3343 (1984); Janyszek, H. and Mrugala, R., Phys. Rev. A 39, 6515 (1989); Janyszek, H., J. Phys. A 23, 477 (1990); Brody, D. and Rivier, N., Phys. Rev. E 51, 1066 (1995).
3. Ruppeiner, G., Rev. Mod. Phys. 67, 605 (1995).
4. Ingarden, R.S., Int. J. Enging. Sci. 19, 1609 (1981); Janyszek, H., Rep. Math. Phys. 24, 1 (1986).
5. Kac, M., Uhlenbeck, G.E., and Hemmer, P.C., J. Math. Phys. 4, 216 (1963).
6. Brody, D.C. and Ritz, A., Nucl. Phys. B 522, 588 (1998).
7. Brody, E.J., Phys. Rev. Lett. 58, 179 (1987).

### TABLE I. The values of the curvature $\mathcal{R}$ ($\pm 0.6$) of the parameter space for the two-dimensional $8 \times 8$ and $16 \times 16$ Ising lattice. The results clearly indicate the phase separation, with a negative curvature phase for low temperatures.

| $8 \times 8$ | $h=0.02$ | 0.18 | 0.34 | 0.50 | 0.66 |
|-------------|---------|-----|-----|-----|-----|
| $T=2.2$    | -2.8    | -9.2 | -4.5 | -5.8 | -0.1 |
| 2.3        | -1.9    | -5.9 | -4.7 | -2.5 | 1.5  |
| 2.4        | +0.6    | -2.8 | -1.2 | -1.4 | +0.1 |
| 2.5        | +1.1    | -2.8 | -1.1 | -1.3 | +0.7 |
| 2.6        | +2.8    | -2.4 | -1.3 | -0.5 | +3.3 |
| 2.7        | +4.1    | -2.5 | -0.7 | -0.2 | +0.2 |
| 2.8        | +5.6    | -1.2 | -0.1 | +0.1 | +1.1 |
| 2.9        | +7.0    | -0.7 | +0.7 | +1.0 | +2.0 |
| 3.0        | +7.3    | +2.4 | +0.1 | +1.5 | +3.0 |

| $16 \times 16$ | $h=0.02$ | 0.18 | 0.34 | 0.50 | 0.66 |
|---------------|---------|-----|-----|-----|-----|
| $T=2.2$       | -58.3   | -7.8 | -5.7 | -2.8 | -2.5 |
| 2.3           | -55.1   | -7.1 | -5.6 | -3.5 | -2.6 |
| 2.4           | -32.4   | -6.4 | -5.3 | -2.4 | -2.1 |
| 2.5           | -6.9    | -2.8 | -2.6 | -1.2 | -0.2 |
| 2.6           | +13.2   | -2.1 | -0.7 | -0.9 | +1.1 |
| 2.7           | +22.1   | +0.9 | -0.8 | -0.1 | +1.6 |
| 2.8           | +24.3   | +1.8 | -1.0 | -0.1 | +2.5 |
| 2.9           | +25.8   | +2.4 | +0.6 | +0.1 | +2.6 |
| 3.0           | +23.9   | +2.9 | +0.7 | +0.3 | +1.3 |