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Geometrical aspects of statistical mechanics

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Investigation of the geometry of thermodynamic state space, based upon the differential geometric approach to parametric statistics developed by Chentsov [*Statistical Decision Rules and Optimal Inference* (*Nauka, Moscow, 1972*)], Efron [Ann. Stat. **3**, 1189 (1975)], Amari [Ann. Stat. **10**, 357 (1982)], and others, provides a deeper understanding of the mathematical structure of statistical thermodynamics. In the present paper, the Riemannian geometrical approach to statistical mechanical systems due to Janyszek [J. Phys. A **23**, 477 (1990)] is applied to various models including the van der Waals gas and magnetic models. The scalar curvature for these models is shown to diverge not only at the critical points but also along the entire spinodal curve. The critical behavior of the curvature derived from the Fisher information metric turns out to coincide with that derived from the entropy differential metric by Ruppeiner [Phys. Rev. A **20**, 1608 (1979)].

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I. INTRODUCTION

Thermodynamics and statistical mechanics provide the basic tools for understanding the observed macroscopic physical world. The geometrical structure of the phase space of statistical thermodynamics was explicitly studied by Gibbs back in the 1870's [6].

In the area of parametric statistics, a number of recent investigations [1–3,7,8] has shown that a useful and illuminating approach to the study of statistical inference consists in regarding a statistical model $\mathcal{M}$ as a differential manifold equipped with a Riemannian metric i_{rs}. A statistical model is a subset of the totality of probability distributions on some fixed sample space, and statisticians assume that a particular model under consideration includes the true distribution of the observed data. The shape of this particular model within the totality of probability distributions, i.e., the geometry of the situation, then plays an important role. This geometry reflects the underlying structure of the physical model described by the distribution. The local properties (mutual distances, flatness, or curvature, etc.) of a statistical model are of especially great interest in the theory of asymptotic inference, and are representable in terms of the above mentioned metric.

The geodesic distance derived from the Riemannian metric i_{rs} (defined below) has been extensively studied for a number of parametric families of probability distributions and interpreted as a measure of dissimilarity of distributions [9]. This distance has also been considered by physicists, and has been referred to in the physical literature as the distinguishability metric [10]. This differential geometric analysis of the relevant parameter space of statistical mechanical models, rather than phase space, has also been pursued in terms of other Riemannian metrics. In 1979, Ruppeiner extended Einstein's theory of fluctuations in order to describe the geometrical structure of thermodynamic parameter space [5] (see also [11]) in terms of the Riemannian metric,

$$g_{rs}=-\frac{\partial^2 H}{\partial\theta^r\partial\theta^s}\ ,$$

where H is the entropy for the thermodynamic model under consideration. This metric was originally introduced by Rao and is known as the entropy differential metric.

In the present paper, we consider the Riemannian geometrical structure for statistical models arising naturally from embedding of the probability density into Hilbert space. That is, one fixes a convenient measure ν (e.g., ν is the Lebesgue measure) on a configuration space, which we denote by $(X,\mathcal{F})$, where X is the sample space (i.e., configuration space) and $\mathcal{F}$ a σ algebra of subset of X [12], and embeds the totality P_ν of the probability measures μ on $(X,\mathcal{F})$, which are absolutely continuous with respect to ν into the unit sphere S of the Hilbert space $L^2(X,\mathcal{F},\nu)$ by the mapping,

$$\mu\to f(\mu)\equiv\left[\frac{d\mu}{d\nu}\right]^{1/2}\ , \tag{1}$$

where $d\mu/d\nu$ denotes the Radon-Nikodym derivative. The unit sphere S is a Hilbertain manifold [13,14] and the Hilbert space norm induces a natural Riemannian metric i on S. If $\{\mu_\theta|\theta\in\mathcal{M}\}\subset P_\nu$ is a family of probability measures parametrized by a smooth finite-dimensional manifold $\mathcal{M}$ and if the mapping

$$\Phi:\mathcal{M}\to S,\Phi(\theta)\equiv f(\mu_\theta) \tag{2}$$

is smooth, then the pull back

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$$i(\theta)=\Phi_\theta^*(i) \tag{3}$$

is a Riemannian metric on $\mathcal{M}$, known as the expected (Fisher) information metric [15].

If we assume that the derivative

$$\frac{d\mu_\theta}{d\nu}=p(x,\theta), x\in X, \theta\in\mathcal{M} , \tag{4}$$

where $p(x,\theta)$ is a probability density which is positive almost everywhere with respect to ν, is a smooth function of θ in the appropriate sense, then the explicit formula for $i(\theta)$ is

$$i_{rs}(\theta_0)=\int \left[\frac{\partial l(x,\theta)}{\partial\theta^r}\frac{\partial l(x,\theta)}{\partial\theta^s}\right]_{\theta=\theta_0} p(x,\theta_0)d\nu(x) , \tag{5}$$

where $l(x,\theta)=\ln p(x,\theta)$ is the log likelihood function and $\{\theta^r\}$ is any admissible local coordinate system on $\mathcal{M}$.

II. STATISTICAL MANIFOLD

In a purely statistical context [3], given a family of probability densities depending smoothly upon a parameter θ and expressible in the form

$$p(x,\theta)=\exp\left[c(x)+\sum_r \theta^r S_r(x)-\psi(\theta)\right] , \tag{6}$$

where the variable x ranges over the sample space, or in physical terminology just the configuration space, the following results are easily verified [3]. Using the integral expression for the quadratic term in Eq. (5), in local coordinates, the Fisher metric tensor is given by

$$i_{rs}(\theta)=-E_p[\partial_r\partial_s l(x,\theta)]=\partial_r\partial_s\psi(\theta) , \tag{7}$$

where $E_p[\cdot]$ denotes the expected value with respect to the probability $p(x,\theta)$ and $\partial_r=(\partial/\partial\theta^r)$. The Christoffel symbols for the metric connection arising from i are

$$\Gamma_{rst}(\theta)=\tfrac{1}{2}\partial_r\partial_s\partial_t\psi(\theta) \tag{8}$$

and the Riemann-Christoffel curvature tensor is, therefore,

$$R_{pqrs}(\theta)=[\Gamma_{rmp}(\theta)\Gamma_{qsn}(\theta)-\Gamma_{rmq}(\theta)\Gamma_{psn}(\theta)]i^{mn}(\theta) . \tag{9}$$

The scalar curvature is defined, as usual, by

$$K=R_{pqrs}i^{ps}i^{qr} , \tag{10}$$

and the expression of this in terms of $\psi(\theta)$ in two dimensions is given in the Appendix.

The tangent space $T_\theta\mathcal{M}$ of the parameter manifold is spanned by the natural basis $\{\partial_r\}=\{\partial/\partial\theta^r\}$, however, it is convenient [3] to deal with the image $\Phi_*(T_\theta\mathcal{M})$ of the tangent space $T_\theta\mathcal{M}$ under the map Φ_* induced by the embedding Φ in Eq. (2). The image of the natural basis is $\{\partial_r l(x,\theta)\}$, and for exponential models of the form given in Eq. (6),

$$\partial_r l(x,\theta)=S_r(x)-\partial_r\psi(\theta) . \tag{11}$$

In the statistical literature, this basis $\{\partial_r l\}$ is usually called the score, and one can also regard the score as a differential 1-form with values in the space of random variables. This differential 1-form is

$$d_p l=\sum_r \frac{\partial l}{\partial\theta^r}(p)d\theta^r , \tag{12}$$

where $l(p)=\ln p$.

In the models of statistical mechanics, we generally deal with Gibbs measures of the form

$$p(x,\theta)=e^{-\sum\theta^r S_r(x)}/Z(\theta) , \tag{13}$$

where the functions $S_r(x)$ determine the form of the action, Z is the partition function, and the parameters $\{\theta^r\}$ are the coordinates of the Riemannian manifold defining the thermodynamic state of the system, which may include temperature, pressure, etc. Thus, in formula (6), we may take $c(x)=0$ and

$$\psi(\theta)=\ln Z(\theta) . \tag{14}$$

From this and the above Eq. (7), if one refers to this ψ or entropy H as the *potential* function for the metric, then for statistical mechanical models, the potential function for the Fisher metric and entropy differential metric are related by the Legendre transformation.

It is interesting to note that Barndorff-Nielsen [8] has established a way to use the observed information matrix j_{rs}, i.e.,

$$j_{rs}(x,\theta)=-\partial_r\partial_s l(x,\theta) ,$$

rather than the expected information $i(\theta)$. His method does not involve an integration over the sample space, as is required in Eq. (5), and he demonstrated the existence of an "observed geometrical structure" paralleling the "expected geometrical structure" given by i. However, in application to statistical mechanics, the probability densities assume the exponential form of Eq. (6), hence $j=i$. Therefore, his approach appears to provide no particular refinements regarding statistical mechanics. However, it might be useful in possible applications of information geometry to quantum mechanics, where the probability densities such as the square of the wave function may not be given by an exponential form.

III. CLASSICAL IDEAL GAS

First, as a fairly trivial example of the Riemannian geometrical representation of statistical mechanics, we shall describe the case of the classical ideal gas.

In this case, we consider a P-T (pressure-temperature) distribution of the form

$$p(q,p,V;\alpha,\beta)=Z^{-1}(\alpha,\beta)\exp[-\beta\mathcal{H}-\alpha V] , \tag{15}$$

where the partition function $Z(\alpha,\beta)$ is

$$Z(\alpha,\beta)=\frac{1}{N!h^{3N}}\int_0^\infty dV\int \exp(-\beta\mathcal{H})dq\,dp\exp(-\alpha V) , \tag{16}$$

$\beta=1/kT$, $\alpha=P/kT$, h is the Planck constant, and N is the number of particles. The Hamiltonian $\mathcal{H}$ is

$$\mathcal{H}=\sum_{i=1}^{N}\frac{p_i^2}{2m}\ , \tag{17}$$

and after integration the partition function becomes

$$Z(\alpha,\beta)=\left[\frac{2\pi m}{h^2\beta}\right]^{3N/2}\alpha^{-(N+1)}\ . \tag{18}$$

Thus, the quantity $\psi(\theta)=\psi(\alpha,\beta)$ for one particle, in the thermodynamic limit, becomes

$$\psi(\alpha,\beta)=\lim_{N\to\infty}N^{-1}\ln Z(\alpha,\beta)=\tfrac{3}{2}\ln\frac{2\pi m}{h^2\beta}-\ln\alpha\ , \tag{19}$$

and the components of the Fisher metric tensor can easily be calculated, with the result

$$i_{rs}=\begin{bmatrix}\alpha^{-2} & 0\\ 0 & \tfrac{3}{2}\beta^{-2}\end{bmatrix}\ . \tag{20}$$

Using the given expression for the scalar curvature (see Appendix), one can also easily calculate that, for a classical ideal gas,

$$K_{\text{cl. ideal gas}}=0\ . \tag{21}$$

This result is also obvious by the following coordinate transformation:

$$\alpha'=\ln\alpha\ ,\quad \beta'=\sqrt{\tfrac{3}{2}}\ln\beta\ ,$$

which takes (20) into the Euclidean metric. Although this result was obtained from P-T distribution, the same result ($K=0$) can be obtained from the usual canonical distribution in which the coordinates are $\beta=1/kT$ and $\alpha=v$, where v is the volume per a particle. Moreover, by solving the geodesic equations for either distribution, one recovers the usual equation of state along adiabatic curves.

IV. van der WAALS GAS

In the previous sections, we have seen how geometrical quantities such as the metric tensor and scalar curvature can be calculated for noninteracting classical particles. Now, we shall examine a case with interactions between classical particles, namely, the van der Waals gas.

Here, we shall again start from the P-T distribution with the partition function,

$$Z(\alpha,\beta)=\frac{1}{N!h^{3N}}\int_{bN}^{\infty}dV\int\exp(-\beta\mathcal{H})dp\,dq\,\exp(-\alpha V)\ , \tag{22}$$

where the Hamiltonian is

$$\mathcal{H}=\sum_{i=1}^{N}\frac{p_i^2}{2m}+\sum_{(ij)}\left[\left[\frac{d}{r_{ij}}\right]^{12}-\left[\frac{d}{r_{ij}}\right]^{6}\right]\ , \tag{23}$$

with $r_{ij}=q_i-q_j$ and d is some constant. After integration over phase space, the partition function becomes

$$Z(\alpha,\beta)=\int_{bN}^{\infty}dV\exp(-\alpha V)z(\beta,V)\ , \tag{24}$$

where

$$z(\beta,V)=\frac{1}{N!}\left[\frac{2\pi m}{\beta h^2}\right]^{3N/2}(V-bN)^N\exp(a\beta N^2/V)\ , \tag{25}$$

is the partition function for the canonical distribution, obtained by the mean field approximation, and a is a positive constant arising from the q integration.

Since the volume integral cannot be calculated exactly, we shall evaluate $\psi(\alpha,\beta)=N^{-1}\ln Z(\alpha,\beta)$ in the limit $N\to\infty$ using the method of steepest decent. Writing the integrand in (24) as

$$\exp(-\alpha V)z(\beta,V)=\exp[Nh(\alpha,\beta,v)]\ ,$$

where $v\equiv V/N$ and

$$h(\alpha,\beta,v)=-\alpha v+\ln\left[\left[\frac{2\pi m}{\beta h^2}\right]^{3/2}(v-b)\right]+\frac{\beta a}{v}\ , \tag{26}$$

$\psi(\alpha,\beta)$ becomes, after taking the limit,

$$\psi(\alpha,\beta)=h(\alpha,\beta,\bar{v})=-\alpha\bar{v}+\ln z(\beta,\bar{v})\ , \tag{27}$$

where $\bar{v}=\bar{v}(\alpha,\beta)$ is a function of α and β, which maximizes $h(\alpha,\beta,v)$, and is the solution of the van der Waals' equation of state given in the Appendix. Since we have obtained a closed form for $\psi(\alpha,\beta)$, although the form of the function $\bar{v}$ is not known, we can calculate the components of the metric tensor i_{rs}, with the result

$$i_{rs}=\begin{bmatrix}-\dfrac{1}{D} & -\dfrac{a/\bar{v}^2}{D}\\[2mm] -\dfrac{a/\bar{v}^2}{D} & \dfrac{3}{2}\dfrac{1}{\beta^2}-\dfrac{(a/\bar{v}^2)^2}{D}\end{bmatrix}\ , \tag{28}$$

where the function $D(\alpha,\beta)$ is defined as

$$D(\alpha,\beta)=\frac{2a\beta}{\bar{v}^3}-\frac{1}{(\bar{v}-b)^2}\ . \tag{29}$$

The scalar curvature for the van der Waals gas can then be calculated, and after some algebra, we obtain

$$K_{\text{v.d.W.}}=\frac{4}{3}\left[\frac{a\beta}{\bar{v}}\right]\frac{F}{D^2}\ , \tag{30}$$

where

$$F(\alpha,\beta)=\frac{a\beta}{\bar{v}^3}-D\ .$$

A more detailed derivation of the metric tensor and the formula used for calculating the scalar curvature is given in the Appendix. The above expression for $K_{\text{v.d.W.}}$ differs from the corresponding result obtained in [4], since the coordinate transformation used for this purpose in [4] was not performed correctly, whereas our result was calculated directly without any coordinate transformation.

From the above expression, $K_{\text{v.d.W.}}$, it is clear that the scalar curvature diverges along $D=0$, i.e., the spinodal curve (see Appendix), which includes the critical point. On the other hand, the system does not return to the same thermodynamic state after following an infinitesimal closed contour around the critical point, or straddling the spinodal curve, and conversely, Maxwell's relation guarantees that any other infinitesimal closed contour is thermodynamically trivial. Thus, we conjecture that divergent curvature is physically characterized by the property of inducing a change in the thermodynamic state of the system $\bar{v}$ upon following an infinitesimal closed contour in the parameter space which encloses a point of divergency.

Also, $K_{\text{v.d.W.}}$ vanishes along the $F=0$ curve, and this sign smoothly changes from positive to negative as one decreases the temperature, in the $(\bar{v},\beta)$ plain.

Note that the P-T distribution with (α,β) as coordinates is used in this section rather than the canonical distribution with $(\bar{v},\beta)$ as coordinates, and this change of thermodynamic parameters is effected through the Legendre transformation in Eq. (27), rather than a coordinate transformation using the equation of the state. The physically meaningful results concerning divergent curvature presented above cannot be obtained in terms of the canonical distribution. An analogous situation occurs in classical mechanics, where canonical transition from Lagrangian variables $(p,\dot{q})$ to Hamiltonian variables (q,p) is only possible through a Legendre transformation, and not through an ordinary coordinate transformation.

V. MAGNETIC MODELS

Magnetic models such as the mean field model or the Ising model are illuminating prototypes of critical phenomena in statistical mechanics or quantum field theory. In this section, we derive an expression for the scalar curvature of the Ising-type mean field model in the lowest order approximation, and also present for comparison the results for the exact one-dimensional Ising model obtained by Janyszek and Mrugala [16].

A. Mean field model

In the mean field model (MFM), interactions between spins are replaced by a field obtained by averaging over all spins. Consider a system of N spins $\{\sigma_i\}$ with the following Hamiltonian:

$$\mathcal{H}=-\frac{qJ}{N-1}\sum_{(ij)}\sigma_i\sigma_j-H\sum_{i=1}^{N}\sigma_i \ , \tag{31}$$

where q is the number of neighbors, J the exchange interaction strength between spins, and H the external magnetic field. The probability density for this model can, therefore, be written as

$$p(\sigma;\alpha,\beta)=\exp[-(kT)^{-1}\mathcal{H}-\psi(\alpha,\beta)] \ , \tag{32}$$

where T is the temperature of the system, and (α,β) can be chosen as $\alpha=H/kT$ and $\beta=J/kT$, respectively. Using the mean field method (see, e.g., Baxter [17] for details), $\psi(\alpha,\beta)$ can be calculated as

$$\psi(\alpha,\beta)=\tfrac{1}{2}\ln\left[\frac{4}{1-M^2}\right]-\tfrac{1}{2}\beta qM^2 \ , \tag{33}$$

where the magnetization $M(\alpha,\beta)$ is given by

$$M=\tanh[\beta qM+\alpha] \ . \tag{34}$$

Expanding this function and substituting into Eq. (33), one obtains

$$\psi(\alpha,\beta)=\tfrac{1}{2}\ln 4-\tfrac{1}{2}\ln\left[1-\left[\frac{\alpha}{1-q\beta}\right]^2\right] -\frac{q}{2}\beta\left[\frac{\alpha}{1-q\beta}\right]^2 , \tag{35}$$

where, for simplicity, only the first term in the expansion of M is considered. Using the formula for the scalar curvature in the Appendix, one can easily calculate that

$$K_{\text{MFM}}=\frac{q}{(q\beta-1)^3} \ . \tag{36}$$

Clearly, this scalar curvature is negative for $\beta<\beta_c$, positive for $\beta>\beta_c$, and diverges at the critical point $\beta_c=1/q$. Owing to the neglect of the higher terms in the expansion of the magnetization in Eq. (34), one loses the information concerning the α dependence of the spinodal curve, which degenerates into a single straight line $\beta=$const. Next, for comparison, we shall present the result for the exact Ising model.

B. The Ising model

For the case of the Ising model, we have

$$p(\sigma;\alpha,\beta)=\exp\left[\beta\sum_{(ij)}\sigma_i\sigma_j+\alpha\sum_{i=1}^{N}\sigma_i-N\psi(\alpha,\beta)\right] , \tag{37}$$

where α and β are defined as in the mean field model, and $\psi=\ln Z$ for the one-dimensional (1D) Ising model is well known to be

$$\psi(\alpha,\beta)=\beta+\ln[\cosh\alpha+(e^{-4\beta}+\sinh^2\alpha)^{1/2}] \ , \tag{38}$$

in the thermodynamic limit. Again, using the same formula in the Appendix, the scalar curvature for the (1D) Ising model becomes

$$K_{\text{1D Ising model}}=\cosh\alpha(\sinh^2\alpha+e^{-4\beta})^{-1/2}+1 \ . \tag{39}$$

See [16] for the components of the metric tensor and other details. The scalar curvature is positive everywhere and diverges at the trivial fixed point $\beta_c=\infty\,(T_c=0)$ with $\alpha=0$.

C. The scaling hypothesis

In the preceding examples, we observed that the scalar curvature diverges along the spinodal curve, which includes the critical point. The critical behavior of thermodynamic quantities such as specific heat can be analyzed by introducing the notion of the scaling, whereby these quantities are described in terms of the reduced temperature $t=T/T_c-1$, and this approach is also applicable to the scalar curvature.

Consider an Ising-type magnetic model with a probability density expressible in the form of Eq. (13),

$$p(\sigma,\theta)=\exp\left[\sum_{r=1}^{2}\theta^r S_r(\sigma)-\psi(\theta)\right].$$

The expected information metric can then be written as

$$i_{rs}=\begin{bmatrix}\langle(\Delta S_1)^2\rangle & \langle(\Delta S_1)(\Delta S_2)\rangle\\ \langle(\Delta S_2)(\Delta S_1)\rangle & \langle(\Delta S_2)^2\rangle\end{bmatrix}, \tag{40}$$

where $\Delta S_i=S_i-\langle S_i\rangle$ and $\langle S_i\rangle$ denotes the mean value of S_i. Using the following formula:

$$\langle(\Delta S_1)^n(\Delta S_2)^m\rangle\sim\int d^dr(t^{1-\alpha})^n(t^\beta)^m\Lambda(rt^\nu)$$
$$=|t|^{n(1-\alpha)+m\beta-d\nu},$$

which is valid when $m+n$ is an even integer and Λ is some scaling function, the behavior of the metric tensor near the critical temperature is as follows:

$$i_{rs}\sim\begin{bmatrix}|t|^{-\alpha} & |t|^{\beta-1}\\ |t|^{\beta-1} & |t|^{-\gamma}\end{bmatrix}. \tag{41}$$

Again, using the formula in the Appendix, the scalar curvature can be written as

$$K=-\frac{1}{2i^2}\begin{vmatrix}\langle(\Delta S_1)^2\rangle & \langle(\Delta S_1)(\Delta S_2)\rangle & \langle(\Delta S_2)^2\rangle\\ \langle(\Delta S_1)^3\rangle & \langle(\Delta S_1)^2(\Delta S_2)\rangle & \langle(\Delta S_1)(\Delta S_2)^2\rangle\\ \langle(\Delta S_1)^2(\Delta S_2)\rangle & \langle(\Delta S_1)(\Delta S_2)^2\rangle & \langle(\Delta S_2)^3\rangle\end{vmatrix}, \tag{42}$$

hence, the behavior of this quantity near the critical temperature is

$$K(t)\sim|t|^{-\kappa}, \tag{43}$$

where $\kappa=2-\alpha$ in terms of the usual critical exponents [18]. This scaling behavior is identical to the one obtained by Ruppeiner [5] although the method is somewhat different. He also pointed out the fact that this critical behavior of the curvature is the inverse of that of free energy. Since $\kappa>0$, this result shows that the scalar curvature diverges at the critical temperature in a more general context than the examples presented in the preceding sections. Note that the scaling law implies that all six terms in the determinant of Eq. (42) have the same critical exponent, and, therefore, detailed calculations of these terms are not necessary in order to derive the result $K\sim|t|^{-\kappa}$ in [4].

VI. CONCLUDING REMARKS

In the previous sections, we have shown through various examples how expected information geometry can be applied to statistical mechanics. However, the usefulness of this approach will remain limited until the emergence of a generally valid physical interpretation of geometrical quantities such as the scalar curvature. In statistics, the usefulness of this geometrical approach is well known, e.g., Edgeworth expansions of estimators, etc. [7,8]. However, these notions have not been applied in theoretical physics.

A number of investigations (see [4,5,11,16] and references cited therein) have been conducted in this direction and the following conclusion has been stated by Janyszek [4], namely, "the scalar curvature diverges at the critical point and the inverse of the scalar curvature K^{-1} is a new quantity to measure the stability of the system." Although this statement does seem plausible, there still exists no rigorous argument showing that the scalar curvature diverges at the critical point. Moreover, as was shown in Sec. IV above, the scalar curvature for the van der Waals gas in the P-T distribution diverges not only at the critical point but also along the spinodal curve, and this is also true for the magnetic models.

However, Eq. (42) shows that the scalar curvature $K(\theta)$ is expressible in terms of second and third order correlation functions, i.e., $K(\theta)$ is a combination of functions which measure the fluctuations of the system, hence, the quantity $K(\theta)$ itself must reflect the fluctuations of the system, which led to the above quoted interpretation of Janyszek. On the other hand, in the simple case of the classical ideal gas, as calculated above, $K(\theta)=0$, whereas other quantities which measure the fluctuations, such as specific heat, do not vanish. Thus, the simple interpretation stated above must be modified.

Divergent curvature implies that the integral of the scalar curvature over the surface bounded by a closed loop (contour) may not vanish in the limit as the size of the loop approaches zero. On the other hand, the thermodynamic state functions of the system, such as mean volume $\bar{v}$ or magnetization M, change when the parameter point θ follows an infinitesimal closed contour surrounding a critical point or straddling the spinodal curve in the parameter space, and, as mentioned in Sec. IV, the spinodal curve is a locus of divergent curvature. This suggests a relation between curvature and nontrivial thermodynamic changes.

From the geometrical viewpoint, curvature can be interpreted as the rotation of a tangent vector after a parallel translation along a closed curve, and the angle of this rotation is the integral of the scalar curvature over the area enclosed by the curve. Therefore, the solution of the open problem of providing a general physical interpretation of the scalar curvature first requires consideration of the physical significance of tangent vectors and parallel transport in statistical manifolds. The problem of providing a rigorous proof that the scalar curvature diverges at critical points (or a counterexample to this conjecture) also remains open. Furthermore, the physical significance of the sign of the curvature is still unknown. It is interesting to note that Ruppeiner proposed the hypothesis that the scalar curvature represents the correlation volume of the thermodynamic system [11]. He also argued that the curvature is a measurement of interactions, however, a general proof of this remains to be an open problem.

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APPENDIX

The derivation of the metric tensor for the van der Waals gas is as follows. The function $\psi(\alpha,\beta)$ was given in Eq. (27) by

$$\psi(\alpha,\beta)=h(\alpha,\beta,\bar{v})=-\alpha\bar{v}+\ln z(\beta,\bar{v}) ,$$

in terms of an unknown function $\bar{v}$. However, we can determine $(\partial\bar{v}/\partial\alpha),(\partial\bar{v}/\partial\beta)$, etc., in the following manner. First, define Ω as

$$\Omega\equiv-\frac{\partial h}{\partial\bar{v}}=\alpha-\frac{1}{\bar{v}-b}+\beta\frac{a}{\bar{v}^2}=0 .$$

The relation $\Omega=0$ is, in fact, the equation of the state for the van der Waals gas. Now, we take the total derivative of Ω,

$$d\Omega=\frac{\partial\Omega}{\partial\alpha}d\alpha+\frac{\partial\Omega}{\partial\beta}d\beta+\frac{\partial\Omega}{\partial\bar{v}}d\bar{v} ,$$

and thus obtain

$$d\bar{v}=-\left[\frac{\partial\Omega}{\partial\alpha}\Big/\frac{\partial\Omega}{\partial\bar{v}}\right]d\alpha-\left[\frac{\partial\Omega}{\partial\beta}\Big/\frac{\partial\Omega}{\partial\bar{v}}\right]d\beta$$
$$=\left[\frac{\partial\bar{v}}{\partial\alpha}\right]d\alpha+\left[\frac{\partial\bar{v}}{\partial\beta}\right]d\beta .$$

Therefore,

$$\frac{\partial\bar{v}}{\partial\alpha}=\frac{1}{D}$$

and

$$\frac{\partial\bar{v}}{\partial\beta}=\frac{a/\bar{v}^2}{D} ,$$

where D is defined by (29).

As is well known the spinodal curve which constitutes the boundary of a semistable region in the parameter space is given by the condition $(\partial\alpha/\partial\bar{v})=0$. Thus, from the above equation, the spinodal curve is given by the condition $D=0$. Using the above results and the chain rule of differentiation, one can easily calculate $i_{rs}=\partial_r\partial_s h$ with the result given in (28).

Although the general expression for the scalar curvature is given by (10), in two dimensions, which is the only case considered in the text, if the metric tensor takes the form as (7), then the scalar curvature assumes the following simple form:

$$K=-\frac{1}{2i^2}\begin{vmatrix}\psi,_{11} & \psi,_{12} & \psi,_{22}\\ \psi,_{111} & \psi,_{112} & \psi,_{122}\\ \psi,_{112} & \psi,_{122} & \psi,_{222}\end{vmatrix} ,$$

where $i=\det(i_{rs})$. All the results concerning the scalar curvature presented in the preceding text are calculated using the above formula.

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