Metricization of thermodynamic-state space and the renormalization group

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We suggest a new geometrical interpretation of the renormalization-group transformation near the critical point. Using the Weinhold-Ruppeiner metricization, conformal Killing symmetry is assumed and scaling laws are verified.

I. INTRODUCTION

This paper is concerned with an intrinsic geometrical interpretation of the scaling properties of a thermodynamic system in the vicinity of a critical point. The metricization of the thermodynamic-state space was carried out in the past; perhaps the subject was treated most exhaustively by Weinhold[1] and Ruppeiner.[2]

In Sec. II we define the Riemannian metric on the space of thermodynamic states and Sec. III discusses a new statistical interpretation of path lengths, while in Sec. IV we introduce the notion of symmetry in our Riemannian space. In particular, in Sec. V we show that the scaling properties usually brought out by renormalization-group procedures are a simple geometrical symmetry and can be derived from the existence of a conformal Killing equation for our metric tensor. While our considerations do not contribute in a substantive way to extending the results of renormalization-group methods, they do provide a new insight into their geometrical meaning.

II. METRIC ON THE SPACE OF THERMODYNAMIC STATES

Consider a homogeneous thermodynamic system depending on $r+1$ extensive state coordinates $\{X^1,X^2,\ldots,X^{r+1}\}$. We shall fix the scale of our system by keeping X^{r+1} fixed. If the homogeneous system characterized by the extensive coordinates $\{X^1,X^2,\ldots,X^r\}$ is not closed but is in contact with a reservoir, then the quantities X^i $(i=1,2,\ldots,r)$ will fluctuate around their equilibrium values.

We can introduce a Riemannian metric tensor g_{ik} $(i,k=1,2,\ldots,r)$ on the manifold of thermodynamic states of our system. Following Ruppeiner's definition[2]

$$g^{ik}(x)=\langle \Delta x^i \Delta x^k\rangle \quad (i,k=1,2,\ldots,r)\,, \tag{2.1}$$

i.e., the contravariant metric tensor is chosen to be equal to the correlation matrix of the fluctuation Δx^i of the coordinates x^i $(i=1,2,\ldots,r)$ defining the thermodynamic state of the system. Because of the transformation properties of a metric tensor, definition (2.1) is valid for arbitrarily chosen coordination of the state space. The x^i can be in particular the extensive coordinates X^i.

Let the entropy S be given as a function of the X's. Since X^{r+1} was fixed, we exclude it from the set of arguments of the function S; hence S will not be a first-order homogeneous function of its arguments. At the points where the system is stable, the matrix constructed from the second partial derivatives of S with respect to the X^i's $(i=1,2,\ldots,r)$ is a negative definite[3] and gives the correlations of the statistically fluctuating X^i's as follows:[4]

$$\langle \Delta X^i \Delta X^k\rangle=-\left[\frac{\partial^2 S(X)}{\partial X \partial X}\right]^{-1}_{ik} . \tag{2.2}$$

From Eqs. (2.1) and (2.2) we get the covariant metric tensor g_{ik} in extensive coordinates (g_{ik} is the inverse of the contravariant matrix g^{ik}):

$$g_{ik}(X)=-\frac{\partial^2 S(X)}{\partial X^i \partial X^k} . \tag{2.3}$$

We can construct a distance[5] ds between two infinitesimally close points of the thermodynamic configurational space, whose coordinates are X and $X+dX$, respectively:

$$(ds)^2\equiv\sum_{i,k=1}^{r} g_{ik}(X)dX^i dX^k=-\sum_{i,k=1}^{r}\frac{\partial^2 S(X)}{\partial X^i \partial X^k}dX^i dX^k . \tag{2.4}$$

This distance ds in the configurational space can be expressed not only by means of the extensive parameters. Introducing the entropic intensive parameters as[3]

$$Y^i=\frac{\partial S(X)}{\partial X^i}\,, \quad i=1,2,\ldots,r \tag{2.5}$$

$(ds)^2$ can be written in the following symmetric form:

$$(ds)^2=-\sum_{i=1}^{r} dX^i dY^i . \tag{2.6}$$

Let us use coordinates Y^i $(i=1,2,\ldots,r)$ in the thermodynamic-state space and define the thermodynamic potential ϕ, which is the Legendre transform of S and is expressed through the Y^i's as

$$\phi=\phi(Y)=S-\sum_{i=1}^{r} X^i Y^i . \tag{2.7}$$

The first derivatives of ϕ give the extensive parameters X:

$$\frac{\partial\phi(Y)}{\partial Y^i}=-X^i\ ,\quad i=1,2,\ldots,r\ . \tag{2.8}$$

Using Eqs. (2.6) and (2.8) one obtains $(ds)^2$ as a function of the intensive parameters:

$$(ds)^2=\sum_{i,k=1}^{r}\frac{\partial^2\phi(Y)}{\partial Y^i\partial Y^k}dY^i dY^k\ . \tag{2.9}$$

From (2.9) we get the metric tensor in intensive coordinates:

$$g_{ik}(Y)=\frac{\partial^2\phi(Y)}{\partial Y^i\partial Y^k}\ ,\quad i,k=1,2,\ldots,r\ . \tag{2.10}$$

III. PATH AND PATH LENGTH

Consider states P_1 and P_2 of the given thermodynamic system and the corresponding points x_1 and x_2 in the space of coordinates. Let us connect x_1 and x_2 by a path. The length of this path is usually defined as the integral of the line element $ds=(\sum g_{ik}dx^i dx^k)^{1/2}$ along the path:[5]

$$l=\int_{x_1}^{x_2}\left[\sum_{i,k=1}^{r}g_{ik}(x)dx^i dx^k\right]^{1/2}\ . \tag{3.1}$$

By varying the path, the minimal path length is called the geodesical distance[5] between points x_1 and x_2.

It is natural to ask[6] what the meaning of the Riemannian distance of two arbitrarily chosen thermodynamic states is. Ruppeiner[2] has constructed a stochastic process in which geodesical distances are relevant quantities. Nevertheless, it seems that this process is not realizable in an obvious way. We are going to show that the global distance derived from Eq. (3.1) corresponds to the so-called statistical distance introduced recently by Wootters[7] as a distance between probability distributions.

Following Wootters, we regard the points x and $x+dx$ along the path as statistically distinguishable if dx is at least equal to the standard fluctuation of x. In terms of the distance (2.4) this is equivalent to $(ds)^2=\sum_{i,k=1}^{r}g_{ik}(x)dx^i dx^k\geq 1$.

Hence the maximal number N of statistically distinguishable states along a given path is equal to the path length (3.1). Varying the trajectory between x_1 and x_2, Wootters interprets the minimum of N as the statistical distance of x_1 and x_2, which is just the geodesical distance on our Riemannian manifold.

IV. SYMMETRIES IN RIEMANNIAN MANIFOLDS (REF. 5)

The metric tensor fully determines the local structure of a Riemannian space. Nevertheless, as is well known, e.g., in general relativity, it is definitely not a trivial task to physically interpret even a known metric tensor. However, there are some properties of the metric which have clear physical consequences: one of them is symmetry.

Consider a point x in the space, the distance of any pair (A,B) of points in the neighborhood of x can be given as

$$(ds_{AB})^2=g_{ik}(x)dx^i_{AB}\,dx^k_{AB}\ , \tag{4.1}$$

where $dx^i_{AB}=x^i_B-x^i_A$, and these distances yield the geometrical structure of the space. From now on, we will use the Einstein convention: There is a summation if the same index occurs twice, above and below.

One can ask if there exists a motion which transforms all these points in such a way that their relative distances remain unchanged up to a common factor, i.e., during this motion, an arbitrary infinitesimal geometrical object remains similar to itself. In the generic case such a motion does not exist; if it does exist, then it means that there is at least one direction in which the geometry does not change, apart from a possible change of scale. Then the motion is called a conformal symmetry.

An infinitesimal motion is defined by a vector field $K(x)$,

$$x^i\to\tilde{x}^i=x^i+\epsilon K^i(x)\ ,\quad i=1,2,\ldots,r \tag{4.2}$$

where ϵ is the infinitesimal parameter of the displacement. Now let us require that the displacement be a conformal symmetry. Then for the new distances

$$(d\tilde{s}_{AB})^2=g_{ik}(\tilde{x})d\tilde{x}^i_{AB}d\tilde{x}^k_{AB} \tag{4.3}$$

we find the relation

$$\exp[\psi(\tilde{x})](d\tilde{s}_{AB})^2=\exp[\psi(x)](ds_{AB})^2 \tag{4.4}$$

with some function ψ characterizing the local scale. Substituting ds_{AB} and $d\tilde{s}_{AB}$ from Eqs. (4.1) and (4.3) one gets

$$\exp[\psi(\tilde{x})]g_{ik}(\tilde{x})d\tilde{x}^i_{AB}\,d\tilde{x}^k_{AB}=\exp[\psi(x)]g_{ik}(x)dx^i_{AB}\,dx^k_{AB}\ . \tag{4.5}$$

Using Eqs. (4.2) and (4.5) and neglecting terms higher than first order in ϵ yields the following equation:

$$g_{ir}K^r_{,k}+g_{kr}K^r_{,i}+g_{ik,r}K^r+hg_{ik}=0\ , \tag{4.6}$$

where $h=\psi_{,r}K^r$. Henceforth the comma followed by an index stands for partial derivative.

Equations (4.6) are called conformal Killing equations and $K^i(x)$ is the conformal Killing vector field of the manifold. That is, the existence of a conformal Killing vector is equivalent to the existence of a conformal symmetry. In the special case when h is a constant function, K is called homothetic motion.

V. RENORMALIZATION-GROUP TRANSFORMATION AS CONFORMAL SYMMETRY

As it is known,[8] the renormalization group expresses certain similarity properties of the states of a given thermodynamic system. Here we are going to formulate this fact in the frame of the Riemannian structure introduced for the state space in Sec. II.

Let us define a change $L\to L/s$ $(s\geq 1)$ of linear scale of a given many-body system. Denoting the renormalization-group element by R_s, the change-of-state coordinate x^i caused by infinitesimal renormalization-group transformation $R_{1+\epsilon}$ can be written as[8]

$$x^i\underset{R_{1+\epsilon}}{\longrightarrow}x^i+\epsilon K^i(x)+O(\epsilon^2)\ . \tag{5.1}$$

The vector field K is the infinitesimal generator of the renormalization group. We claim that K satisfies the special conformal Killing equation [see Eq. (4.6)]

$$g_{ir}K^r_{,k}+g_{kr}K^r_{,i}+g_{ik,r}K^r+dg_{ik}=0 \tag{5.2}$$

in the vicinity of the critical point, where d is the number of spatial dimensions of the system.

Let us verify that if K is computed from a renormalization group via Eq. (5.1) then the conformal-symmetry assumption (5.2) yields the usual critical behavior.

Consider a ferromagnetic system possessing two relevant parameters, temperature T and external magnetic field H. If we choose $x=(x^1,x^2)=(T,H)$ as coordinates of the thermodynamic states, we get a Riemannian metric (2.1) in the following form:

$$\begin{bmatrix} g_{TT} & g_{TH} \\ g_{HT} & g_{HH} \end{bmatrix} = \begin{bmatrix} CT^{-2} & M_{,T}T^{-1} \\ M_{,T}T^{-1} & \chi T^{-1} \end{bmatrix}, \tag{5.3}$$

where C, M, and χ stand for specific heat, magnetization, and susceptibility, respectively.

Let us choose for simplicity the renormalization-group transformation in such a way that, other than the temperature and the magnetic field, no more "coupling constants" are generated in the course of the transformation (e.g., one-dimensional Ising model, Migdal-Kadanoff transformation[9]). In this case one can write the infinitesimal generator K of the renormalization group in the neighborhood of the critical point $x_c=(T_c,0)$ as

$$\begin{aligned} &K^1=K^T=A\,|\tau|\ , \quad \text{where } \tau=T-T_c \\ &K^2=K^H=B\,|H|\ , \quad A,B \text{ constant}\ . \end{aligned} \tag{5.4}$$

Substituting expression (5.4) of the vector field K into the Killing equation (5.2) we get the following three differential equations for the components of the metric tensor:

$$\begin{aligned} &2Ag_{TT}+A\,|\tau|\,g_{TT,T}+B\,|H|\,g_{TT,H}=-dg_{TT}\ , \\ &2Bg_{HH}+B\,|H|\,g_{HH,H}+A\,|\tau|\,g_{HH,T}=-dg_{HH}, \\ &(A+B)g_{TH}+A\,|\tau|\,g_{TH,T}+B\,|H|\,g_{TH,H}=-dg_{TH}\ . \end{aligned} \tag{5.5}$$

We conclude from these equations that the components of the metric tensor are generalized homogeneous functions in the neighborhood of the critical point:

$$\begin{aligned} &g_{TT}(\lambda^A\tau,\lambda^B H)=\lambda^{-d-2A}g(\tau,H)\ , \\ &g_{TH}(\lambda^A\tau,\lambda^B H)=\lambda^{-d-A-B}g(\tau,H)\ , \\ &g_{HH}(\lambda^A\tau,\lambda^B H)=\lambda^{-d-2B}g(\tau,H)\ . \end{aligned} \tag{5.6}$$

From Eqs. (5.3) and (5.6) one can easily derive the critical behavior of the quantities of experimental interest:

$$\begin{aligned} &C\sim g_{TT}(\tau,0)\sim |\tau|^{-d/A-2}\ , \\ &M_{,T}\sim g_{TH}(\tau,0)\sim |\tau|^{-d/A-1-B/A}\ , \\ &\chi\sim g_{HH}(\tau,0)\sim |\tau|^{-d/a-2B/A}\ , \\ &M^{cr}_{,H}\sim g_{HH}(0,H)\sim |H|^{-d/B-2}\ . \end{aligned} \tag{5.7}$$

Using the standard definitions for the critical indices,[10] one gets the following expressions for the critical exponents of the specific heat, spontaneous magnetization, susceptibility, and critical magnetization, respectively:

$$\begin{aligned} &\alpha=2+d/A\ , \\ &\beta=-d/A-B/A\ , \\ &\gamma=2B/A+d/A\ , \\ &1/\delta=-d/B-1\ . \end{aligned} \tag{5.8}$$

From (5.8) the usual scaling laws follow, if d is indeed the dimensionality of the space.

Let us summarize our geometrical interpretation of the similarities during renormalization. Choose three neighboring states near the critical point and perform a renormalization-group transformation for them, with the same parameter s. Then, the triangle formed by the three states in the parameter space remains similar after the transformation, because the ratios of the lengths of the sides, measured by the expectation values of the fluctuations as units, remain unchanged as a consequence of the conformal Killing equation.

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