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ABSTRACT

After introducing a suitable Riemannian metric in thermodynamic state space, with a simple statistical thermodynamic interpretation, we show that the existence of scaling must imply the existence of a conformal Killing vector field in the neighborhood of a critical point.

АННОТАЦИЯ

В пространстве термодинамических состояний накладывается риманова метрика, допускающая простую статистическую термодинамическую интерпретацию. Показано, что из существования скэйлинга следует существование конформного векторного поля Киллинга в окрестности критической точки.

KIVONAT

Termodinamikai állapottéren egyszerü statisztikus termodinamikai interpretációval rendelkező Riemann-metrikát vezetünk be. Megmutatjuk, hogy a szkéling létezéséből következik egy konformis Killing-vektormező létezése kritikus pont környezetében.

1. 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 has been carried out in the past; perhaps the subject has been treated most exhaustively by Weinhold[1] in a recent series of papers. Unlike Weinhold[1] and the references cited in his papers, we wish to focus more ditectly on the relationship between Euclidean spaces defined by different thermodynamic states as a differentiable manifold obtained after introducing local vector space. The particular choice of metric we make (see the next section) has a particularly simple statistical thermodynamic interpretation (see Section 3). Having defined the metric, in section 4 we introduce the notion of symmetry in our Riemannian space. In particular in the last section we show that the scaling properties brought out by renormalization group procedures are a simple geometrical symmetry which implies the existence of a conformal Killing equation for our metric tensor.

While our considerations do not contribute in a substansive way to extend the results of renormalization group methods they do provide a general insight into their geometric meaning.

2. METRIC ON THE SPACE OF THERMODYNAMIC STATES

Consider a homogeneous thermodynamic system having r+1 degrees of freedom, the $X_1, X_2 \ldots X_{r+1}$ extensive state coordinates, and let the entropy S be given as the function of the X's. We shall consider our system as a closed one in the following sense: we shall keep X_{r+1} fixed excluding it from the 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, is a negative definite.[2,3] By means of this matrix we can introduce a distance ds between two infinitesimally close points of the thermodynamic (configurational) space, whose coordinates are X and X+dX respectively:

$$(ds)^2 = - \sum_{i,k=1}^{r} \frac{\partial^2 S(X)}{\partial X_i \partial X_k} dX_i dX_k \quad . \tag{2.1}$$

This distance ds in the configurational space can be expressed not only by means of the extensive parameters; but introducing the (entropical) intensive parameters as

$$Y_i = \frac{\partial S(X)}{\partial X_i} \quad , \tag{2.2}$$

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

$$(ds)^2 = - \sum_{i=1}^{r} dX_i dY_i \quad . \tag{2.3}$$

Let us use Y's coordinates in the thermodynamic space and let us define the thermodynamic potential ϕ, which is the Legendre-transform of S and is expressed through the Y_i's as

$$\phi = \phi(Y) = S - \sum_{i=1}^{r} X_i Y_i \quad . \tag{2.4}$$

The first derivatives of ϕ give the extensive parameters X:

$$\frac{\partial\phi(Y)}{\partial Yi} = -X_i \quad . \tag{2.5}$$

Using (2.3) and (2.5) we obtain $(ds)^2$ as a function of the intensive parameters:

$$(ds)^2 = \sum_{i,k=1}^{r} \frac{\partial^2\phi(Y)}{\partial Y_i \partial Y_k} dY_i dY_k \quad . \tag{2.6}$$

Let us also investigate the general case when the state is described by mixed coordinates, for example, X_α extensive and $Y_{\alpha'}$ intensive parameters where $\alpha = 1,2,\ldots,k$ and $\alpha' = k+1,\ldots,r$. In this case it is convenient to introduce the potential

$$\phi' = \phi'(X_1 \ldots X_k, Y_{k+1}, \ldots Y_r) = S - \sum_{\alpha'} Y_{\alpha'} X_{\alpha'} \tag{2.7}$$

whose first derivatives are

$$\frac{\partial\phi'}{\partial X_\alpha} = Y_\alpha \;, \; \frac{\partial\phi'}{\partial X_{\alpha'}} = - X_{\alpha'} \quad . \tag{2.8}$$

Substituting (2.8) into (2.3)

$$(ds)^2 = - \sum_{\alpha\,\beta} \frac{\partial^2\phi'}{\partial X_\alpha \partial X_\beta} dX_\alpha dX_\beta + \sum_{\alpha',\beta'} \frac{\partial^2\phi'}{\partial Y_{\alpha'} \partial Y_{\beta'}} dY_{\alpha'} dY_{\beta'} \quad . \tag{2.9}$$

Here α and β' take the same values as α and α' respectively. It is interesting to note that mixed terms of the type dXdY do not appear in (2.9).

Having introduced ds as the infinitesimal distance the space of stable states of the homogeneous, closed, equilibrium thermodynamic system can be considered as an r-dimensional Riemannian manifold[4] with distance ds. The metric tensor of this Riemannian manifold, expressed through the extensive coordinates is

$$g_{ik} = -S,_{ik} \equiv - \frac{\partial^2 S}{\partial X_i \partial X_k} \quad . \tag{2.10}$$

In intensive coordinates

$$g_{ik} = \phi,_{ik} \equiv \frac{\partial^2 \phi}{\partial Y_i \partial Y_k} \quad , \tag{2.11}$$

and using mixed coordinates

$$g_{ik} = \begin{cases} -\phi',_{ik} & \text{if both the i'th and k'th coordinates are extensive,} \\ \phi',_{ik} & \text{if both the i'th and k'th coordinates are intensive,} \\ 0 & \text{otherwise.} \end{cases} \tag{2.12}$$

The general coordinates introduced in the thermodynamic space, in what follows will be denoted by $x = (x^1, x^2, \ldots, x^r)$ as in the formalism of General Relativity. When we make a transformation from one coordinate system to another the g_{ik} matrix will be transformed as a tensor. In a given coordinate system, the invariant distance ds can be written as

$$ds^2 = g_{ik}(x)\, dx^i dx^k \equiv \sum_i \sum_k g_{ik}(x) dx^i dx^k \quad . \tag{2.13}$$

In what follows the Einstein summation convention is used, that is the summation sign over repeated indeces will not be written out explicitly. If we have two points x_1 and x_2 (not necessarily close to each other) and a continuous curve connecting them, the length of this curve is defined as

$$\int_{x_1}^{x_2} ds = \int_{x_1}^{x_2} (g_{ik}dx^i dx^k)^{1/2} \tag{2.14}$$

where the integrals are taken along the curve. In Riemannian Geometry the distance between the pair of points x_1 and x_2 is defined as

$$s(x_1,x_2) \equiv \min \int_{x_1}^{x_2} ds \tag{2.15}$$

and the minimizing curve is called the geodesic between x_1 and x_2.

3. STATISTICAL INTERPRETATION OF THE METRIC

If the homogeneous thermodynamic system, characterized by the $X_1,\ldots.X_r$ extensive coordinates is not closed but is a part of a homogeneous system which is much greater in size then the system in question, then the quantities X will fluctuate around their equilibrium values. The thermodynamic fluctuation δX in quadratic approximation follows the Gaussian distribution[5]:

$$P(\delta X) \sim \exp\{\frac{1}{2} \sum_{ik=1}^{r} \frac{\partial^2 S(X)}{\partial X_i \partial X_k} \delta X_i \delta X_k\} . \tag{3.1}$$

In the exponent of Eq. (3.1) we have the squared distance $(ds)^2$ of the Riemannian metric introduced in Sec. 2. According to (2.1) the probability of fluctuations around a given state of the system (at least in the quadratic approximation in the variation of the coordinates) depends only on the distance ds represented by the fluctuation:

$$P(\delta X) \sim \exp\{-\frac{1}{2}(ds)^2\}. \tag{3.2}$$

Since in Riemannian manifolds the choice of coordinates does not affect the value of ds we can use the general coordinates x^i, i=1 ... r . Following (2.13) we can write (3.1) in general coordinates as

$$P(\delta x) \sim \exp \{- \frac{1}{2} g_{ik} \delta x^i \delta x^k\} . \qquad (3.3)$$

Let us make explicit the relationship between the fluctuations and the metric tensor. According to (3.2) the average of the squared distance $(ds)^2$ represented by the fluctuations is unity (if $P(\delta X)$ is normalized to unity):

$$\overline{(ds)^2} = g_{ik} \overline{\delta x^i \delta x^k} = 1 \qquad (3.4)$$

whence

$$\overline{\delta x^i \delta x^k} = g^{ik} , \qquad (3.5)$$

consequently the correlation matrix of the fluctiations of the coordinates of a thermodynamic state is a tensor and is identical to the metric tensor, introduced earlier. This is the statistical content of the metric introduced in Sec. 2 and we could have equally well chosen Eg. (3.5) instead of the formal thermodynamic definition used in the previous section. Note that (3.5) is valid for an arbitrary choice of coordinates on the space of states.

It is a natural question to ask what is the meaning of the distance (2.15) between two arbitrary thermodynamic states. We are going to show that the global distance (2.15) corresponds to the so called statistical distance introduced recently by Wootters[6] as a distance between probability distributions. Let us consider states P_1 and P_2 of the given thermodynamic system and the corresponding x_1 and x_2 points in the space of the coordinates. Let us connect x_1 and x_2 by a continuous curve in this space. Now we estimate how many well distinguishable states this curve goes through and let us denote this number by N. Following Wootters[6] we consider the points x and x+dx along this curve statistically distinguishable if dx is equal to (or greater than) the standard fluctuation of x, that is $(ds)^2 = g_{ik}dx^i dx^k = 1$. This means, that N is equal to the length (2.14) of the curve connecting P_1 and P_2. Wootters[6], varying the trajectories between x_1 and x_2 interprets the minimum of N as the statistical distance of x_1 and x_2, which, according to (2.15) is equal to the distance on the Riemannian manifold introduced by us earlier.

4. SYMMETRIES

The metric tensor fully determines the local structure of a Riemann space, nevertheless, as it 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 (if symmetries exist in the investigated space).

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

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

where $dx^i_{AB} = x^i_B - x^i_A$, and these distances yield the structure of the space. One can ask if there exists a motion which transforms all these points in such a way that the distances remain unchanged.

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, and then the motion is called a symmetry.

An infitesimal motion is defined by a vector field K^i,

$$\tilde{x}^i = x^i + K^i(x)\varepsilon \qquad (4.2)$$

where ε is the (infinitesimal) parameter of the displacement. Now let us require that the displacement be a symmetry. Then from (4.1)

$$d\tilde{s}^2 = ds^2 , \qquad (4.3)$$

i.e.

$$g_{ik}(\tilde{x})d\tilde{x}^i_{AB}d\tilde{x}^k_{AB} = g_{ik}(x)dx^i_{AB}dx^k_{AB} \quad . \qquad (4.4)$$

Calculating the coordinate differences at the new points, and using eq. (4.2) one gets:

$$\begin{aligned} g_{ik}\,(x + K(x)\varepsilon)(x^i_B + \varepsilon K^i(x_B) - x^i_A - \varepsilon K^i(x_A)) \times \\ (x^k_B + \varepsilon K^k(x_B) - x^k_A - \varepsilon K^k(x_A)) = \qquad (4.5) \\ = g_{ik}(x)(x^i_B - x^i_A)(x^k_B - x^k_A) \; . \end{aligned}$$

Since ε is infinitesimal, one should keep only the ε^o and ε terms in eq. (4.5). The first nontrivial term is of the order of ε, whence one gets that condition (4.3) is fulfilled if and only if

$$g_{ir}K^r{}_{,k} + g_{kr}K^r{}_{,i} + g_{ik,r}K^r = 0 \quad . \qquad (4.6)$$

Eqs. (4.6) are called Killing equations[7] and K^i is the Killing vector of the space. That is, the existence of a Killing vector is equivalent to the existence of a symmetry direction.

Eq. (4.6) has been obtained from the condition that the transformed geometric objects remain completely unchanged. Requiring a weaker condition that they remain similar in a geometric sense, i.e. there may be a change of scale,

$$e^{\psi(\tilde{x})} \, d\tilde{s}^2_{AB} = e^{\psi(x)} \, ds^2_{AB} \tag{4.7}$$

one gets the conformal Killing equation[7]

$$g_{ir}K^{r}{}_{,k} + g_{kr}K^{r}{}_{,i} + g_{ik,r}K^{r} + h\, g_{ik} = 0 \tag{4.8}$$

where

$$h = \psi_{,r}K^{r} \; . \tag{4.9}$$

If a symmetry exists, one can always use such a coordination of the space that the metric tensor is independent of the first coordinate. For conformal symmetries there exist coordinates in which g_{ik} contains the first one only in a multiplicative factor:

$$g_{ik}(x) = e^{-\psi(x^1, x^2 \ldots)} \, g^{(0)}_{ik}(x^2 \ldots) \; . \tag{4.10}$$

In the special case when h in eqs. (4.9) - (4.11) is a constant,

$$\psi = \psi(x) = h\, x^1 \; . \tag{4.11}$$

5. SCALING AS GEOMETRICAL SYMMETRY

It is generally accepted that the physical system obeys some scaling laws in the vicinity of the critical point[1], of a higher order phase transition. This means that approaching the critical point the system goes through similar states; the only changes occur in the scales of the parameters of the system[2].

In the Riemannian space of states introduced in Sect. 2. such similarities appear as geometrical similarities thus, according to Sect. 4, the existence of scaling must imply the existence of some Killing vector field (being the mathematical consequence of geometrical similarity) in the neighborhood of the critical point.

In what follows we show, that the usual version of scaling, namely the assumption that the thermodynamic potentials are generalized homogeneous functions of their arguments[8] indeed leads to a <u>special conformal</u> Killing vector field. Let us chose ϕ, defined by (2.4) as the thermodynamic potential. Then the homogeneity condition can be written[2] as

$$\phi(\lambda^{a_i} y^i) = \lambda\phi(y^i) \quad i=1,2\ldots r \quad . \tag{5.1}$$

Here $y^i = Y_i - Y_{i(crit)}$ and a_i are related to the usual critical indeces[2]. (5.1) is assumed to be an identity in λ. Thus upon differentiating eq. (5.1) with respect to λ and setting $\lambda=1$, one gets

$$\sum_{i=1}^{r} a_i y^i \phi_{,i} = \phi \quad . \tag{5.2}$$

By introducing a vector field

$$K^i(Y) = d a_i y^i \ , \tag{5.3}$$

where d is the number of spatial dimensions of the system, eq. (5.2) can be written as

$$K^r \phi_{,r} - d\phi = 0 \ . \tag{5.4}$$

By differentiating this equation twice with rexpect to the y^i, and using (2.11) and (5.3) for the definities of the metric tensor one obtains

$$g_{ir}K^r{}_{,k} + g_{kr}K^r{}_{,i} + g_{ik,r}\,K^r - dg_{ik} = 0 \qquad (5.5)$$

which is the special conformal Killing equation introduced in (4.8). It should be noted that (5.5) is valid only asymptotically in the vicinity of the critical point.

The coefficient a_i in eq. (5.2) can be calculated from the fixed point equations of the renormalization group[8]. One can easily show that the vector field, defined by (5.3) is just the infitesimal generator of the renormalization group transformation near the critical point. That is if

$$(y^i)' = R^i_s(y) \qquad (5.6)$$

then

$$K^i(y) = \frac{d}{ds} R^i_s(y)\Big|_{s=1+0} \quad . \qquad (5.7)$$

Here R_s denotes the operator of the renormalization group transformation corresponding to a scale parameter s. The meaning of s is the following: By using a renormalization group transformation one wants to eliminate successively degrees of freedom from the system in the hope that one finally obtains a system with fewer number of degrees of freedom. This transformation, in order to preserve the physical properties of the original system must leave the total free energy and the density of the degrees of freedom invariant. In other words if from now on $\phi(Y)$ and $\phi(Y')$ are the ϕ potentials per one degree of freedom of the original and transformed systems respectively and N and N′ are the number of degrees of freedom in the original and transformed system respectively then

$$N\phi(y) = N'\phi(y') \;, \tag{5.8}$$

$$N/L^d = N'/(L')^d \tag{5.9}$$

should hold, where L^d and $(L')^d$ denote the volume element of the original and transformed systems respectively. Since $N'<N$, (5.9) defines a scale transformation

$$L' = s^{-1}L \tag{5.10}$$

where $N'/N = s^{-1}<1$. Then (5.8) implies

$$\phi((y^i)') = \phi(s^{\lambda_i}y^i) = s^d\phi(y^i) \tag{5.11}$$

where

$$(y^i)' = s^{\lambda_i}y^i \tag{5.12}$$

is the linearized form (near to the critical point) of (5.6) and the λ_i are the eigenvalues of the linearized renormalization group transformation[8]. Now we can easily prove our statement (5.7) about the K vector field. Let us expand (5.6) around s=1 (the identity transformation)

$$(y^i)' = y^i + \left.\frac{\partial R}{\partial s}\right|_{s=1} \varepsilon \tag{5.13}$$

where $\varepsilon = s-1$. Now from the definition (4.2) one gets immediately (5.7). Also, on comparing (5.3) with (5.11) one obtains

$$a_i = \lambda_i/d \quad . \tag{5.14}$$

So we conclude that the existence of a fixed point of the renormalization group transformation, describing a higher order phase transition, implies a special conformal Killing equation for the metric tensor which was introduced. The corresponding Killing vector is the infinitesimal generator of the renormalization group transformation, which then vanishes at the fixed point (see eq. (5.3)).

Eqs. (5.5) renders a clear geometrical interpretation for the renormalization group transformation. 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 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, which is the consequence of the Killing equation (5.5)[7].

The existence of scaling laws, characteristic for the behaviour near the critical point, follows from (5.5). To demostrate this simply take a system with a single intensive parameter. In this case $y \sim (T-T_c)$, (T is the temperature), and the only element of the metric tensor $g \sim g_{11} \sim C$, where C is the specific heat with $C \sim y^{-\alpha}$ close to the critical point. In this case (5.5) leads to

$$2g \frac{dK}{dy} + \frac{dg}{dy} K - dg = 0 \qquad (5.15)$$

using $g \sim y^{-\alpha}$, $K = \frac{1}{\nu} y$, where ν is the correlation length exponent[8] defined by

$$y' = s^{1/\nu} y \,, \qquad (5.16)$$

one gets from (5.15)

$$2 - \alpha = d\nu \qquad (5.17)$$

which is a well-known scaling law[2].

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