PHYSICAL REVIEW A VOLUME 39, NUMBER 12 JUNE 15, 1989

Riemannian geometry and the thermodynamics of model magnetic systems

H. Janyszek and R. Mrugała
Institute of Physics, Nicholas Copernicus University, 87-100 Toruń, Poland
(Received 12 September 1988)

A Riemannian metrical structure of the parameter space has been introduced and investigated for magnetic systems described in the framework of quantum statistics. The introduced metric is based on the conception of the relative information. Two contrasting models have been investigated in detail: the one-dimensional Ising model, with short-range interactions, and the mean-field model of Kac, with long-range interactions. In the second case the metric tensor degenerates. The degeneration has been removed by adding the lattice energy to the original magnetic Hamiltonian. It turns out that in both cases the scalar curvature of parameter space tends toward plus infinity while approaching the critical points. The inverse of the scalar curvature, given by the second and third moments of stochastic variables, has been interpreted as a measure of the stability of the considered magnetic systems. The scalar curvature represents a joint part of fluctuations caused by the interactions of spins.

I. INTRODUCTION

Recently many authors[1-5] have investigated the structure of the state space of thermodynamic parameters in the framework of Riemannian geometry. In our previous papers[6,7] we investigated from this point of view various classical and quantum-fluid systems. It has turned out that the Riemannian scalar curvature R of the parameter space is especially important. Statistically, R depends on the second and third moments of fluctuations or on the second and third derivatives of the partition function. Phenomenologically R is expressed through the second and third derivatives of an appropriate thermodynamic potential function. The behavior of R is very interesting in the vicinity of the critical point and singular at this point. That is why we proposed to interpret R as a measure of the stability of thermodynamic systems.

In this paper we extend these geometrical methods to simple magnetic systems. We start with the one-dimensional (1D) Ising model, for which it is possible to calculate all quantities exactly. Next, we investigate the mean-molecular-field approximation and its extension by taking also into account the thermal energy of the lattice. We show that such extension is necessary because of some requirements of a geometrical nature.

II. RIEMANNIAN GEOMETRY OF THE PARAMETER SPACE

In order to introduce a Riemannian structure into the space of thermodynamic parameters, we start from an equilibrium density operator

$$\rho = Z^{-1}(\beta) e^{-\beta^i F_i}, \quad i = 1,2,\ldots,r \tag{2.1}$$

(the summation over repeated indices is assumed). As usual the series $F_1, F_2, \ldots, F_r$ stands for a set of self-adjoint linearly independent (but not, in general, statistically independent) operators which describe our system and $\beta = (\beta^1, \beta^2, \ldots, \beta^r)$ are classical real parameters (statistical temperatures) which characterize the environment of the system. $Z(\beta)$ is the partition function, i.e.,

$$Z(\beta) = \mathrm{Tr} e^{-\beta^i F_i} . \tag{2.2}$$

Physically, F_i represents quantities whose numerical values may fluctuate around their mean values $m_i = \langle F_i \rangle = \mathrm{Tr}(\rho F_i)$. On the contrary, β^i do not fluctuate and their numerical values are fixed according to the state environment. Any change in the state of environment invokes changes of ρ and m_i. Therefore we will treat ρ in (2.1) as an r-parameter family of the density operators.

For quantum systems, F_i do not necessarily commute. This causes some inconvenience in defining metric structures on the parameter space. Some quantities which are equivalent for commuting F_i may be different for non-commuting F_i. For classical systems, we defined the metric tensor in the following way. At first we took the microscopic entropy as operator

$$s = -\ln\rho = \beta^i F_i + \ln Z(\beta) , \tag{2.3}$$

which was treated as a vector in $(r+1)$-dimensional space with axes labeled by F_i and $F_0 = 1$, and with β^i and $\ln Z(\beta)$ as components of the vector. Then the distance in the parameter space was defined as

$$dl^2 = \langle (ds)^2 \rangle = \langle (d \ln\rho)^2 \rangle = \left\langle \frac{\partial \ln\rho}{\partial \beta^i} \frac{\partial \ln\rho}{\partial \beta^j} \right\rangle d\beta^i d\beta^j , \tag{2.4}$$

where dl is the line element and $\langle \cdots \rangle = \mathrm{Tr}\rho(\cdots)$ denotes the mean value. Consequently, the metric tensor was

$$g_{ij}(\beta) = \left\langle \frac{\partial \ln\rho}{\partial \beta^i} \frac{\partial \ln\rho}{\partial \beta^j} \right\rangle . \tag{2.5}$$

The present approach to the metrization in quantum-statistical mechanics is more physically justified than the metric introduced by Wootters.[8] In the Wootters work were accepted all probability distributions. We consider only physically interesting distributions given by (2.1), so that we have an r-dimensional space. Definition (2.5) is unacceptable in the case of noncommuting operators F_i because $\partial \ln\rho/\partial\beta^i$ and $\partial \ln\rho/\partial\beta^j$ do not commute. The simplest solution seems to be in the symmetrical form of (2.4), when for g_{ij} we put

$$g_{ij}(\beta)=\tfrac{1}{2}\left[\left\langle \frac{\partial \ln\rho}{\partial\beta^i}\frac{\partial \ln\rho}{\partial\beta^j}\right\rangle+\left\langle \frac{\partial \ln\rho}{\partial\beta^j}\frac{\partial \ln\rho}{\partial\beta^i}\right\rangle\right] . \tag{2.6}$$

We will, however, abandon the definition (2.6) because it does not have any clear thermodynamic interpretation; in particular, g_{ij} given by (2.6), does not have an obvious link with the thermodynamic theory of fluctuations.[2,9]

In this paper we will adopt another definition of the metric tensor in the form discussed by Ingarden *et al.*[10] Let us consider two close statistical states: $\rho=\rho(\beta)$ and $\sigma=\rho(\beta+d\beta)$. According to Umegaki,[11] we define the information distance between these two states (information gain, relative entropy) as

$$\begin{aligned} I(\rho|\sigma)&=\mathrm{Tr}[\rho(\ln\rho-\ln\sigma)]=\mathrm{Tr}[\rho(-s+s')]\\ &=\langle \Delta s\rangle_\rho \geq 0 , \end{aligned} \tag{2.7}$$

where $s'=-\ln\sigma$, $\Delta s=s'-s$, and the subscript ρ indicates the averaging with ρ. Δs may be treated as a difference of two vectors of the type (2.3). Because $I(\rho|\sigma)$ is, in general, different from $I(\sigma|\rho)$, we will take further the symmetrical information distance I_s:

$$I_s=I(\rho|\sigma)+I(\sigma|\rho)=\langle\Delta s\rangle_\rho-\langle\Delta s\rangle_\sigma\geq 0 . \tag{2.8}$$

The Riemannian structure of the space of parameters $\beta^1,\dots,\beta^r$ we define now by means of the formula[10]

$$dl^2=I_s=I(\rho(\beta+d\beta)|\rho(\beta))+I(\rho(\beta)|\rho(\beta+d\beta)) . \tag{2.9}$$

Next we expand (2.9) into a power series in the neighborhood of β, up to second-order terms in $d\beta$. In this approximation, first and second terms of (2.9) lead to the same result. In order to calculate information distance, one has to use the well-known Wilcox[12] formula for the parameter differentiation of an exponential operator

$$\frac{dl^{A(\mu)}}{d\mu}=\int_0^1 d\lambda\, e^{(1-\lambda)A}\frac{dA}{d\mu}e^{\lambda A}=\int_0^1 d\lambda e^{\lambda A}\frac{dA}{d\mu}e^{(1-\lambda)A} . \tag{2.10}$$

One can easily show that

$$I_s(\rho|\rho)=0 , \quad \left.\frac{\partial I_s}{\partial\beta^i}\right|_\beta=0 , \quad i=1,2,\dots,r \tag{2.11}$$

while for ρ given by

$$\frac{1}{2}\frac{\partial^2 I_s}{\partial\beta^i\partial\beta^j}=\int_0^1 d\lambda\,\mathrm{Tr}\left[\rho e^{\lambda\beta^l F_l}\frac{\partial\ln\rho}{\partial\beta^i}e^{-\lambda\beta^l F_l}\frac{\partial\ln\rho}{\partial\beta^j}\right]=\int_0^1 d\lambda\,\mathrm{Tr}[\rho e^{\lambda\beta^l F_l}(F_i-\langle F_i\rangle)e^{-\lambda\beta^l F_l}(F_j-\langle F_j\rangle)] . \tag{2.12}$$

This may be further written in the form

$$\frac{1}{2}\frac{\partial^2 I_s}{\partial\beta^i\partial\beta^j}=\frac{\partial^2 \ln Z}{\partial\beta^i\partial\beta^j}=-\left\langle\frac{\partial^2\ln\rho}{\partial\beta^i\partial\beta^j}\right\rangle . \tag{2.13}$$

Finally the (local) square distance in the parameter space is given by

$$dl^2=g_{ij}(\beta)d\beta^i d\beta^j , \quad g_{ij}=\frac{\partial^2 \ln Z}{\partial\beta^i\partial\beta^j}=-\left\langle\frac{\partial^2\ln\rho}{\partial\beta^i\partial\beta^j}\right\rangle . \tag{2.14}$$

For classical systems, i.e., for commuting F_i, both definitions (2.6) and (2.14) are equivalent. This is, however, not the case for quantum systems. Some insight into the differences of these two metrics gives a comparison of those parts of (2.4) and (2.9) which are expressed through s.

Our choice of the metric (2.14) is motivated by physical arguments, statistical and phenomenological. Statistically, the components of (2.14) are given by the covariances of two operators F_i and F_j, where by the covariance of F_i and F_j we mean

$$\mathrm{cov}(F_i,F_j)=\int_0^1 d\lambda\,\mathrm{Tr}[\rho e^{\lambda\beta^l F_l}(F_i-\langle F_i\rangle)e^{-\lambda\beta^l F_l}(F_j-\langle F_j\rangle)] . \tag{2.15}$$

This definition of covariances makes sense because, for commuting F_i, it reduces to the classical expression for the covariances

$$\mathrm{cov}(F_i,F_j)=\langle(F_i-\langle F_i\rangle)(F_j-\langle F_j\rangle)\rangle . \tag{2.16}$$

Phenomenologically, g_{ij} are expressed through the second derivatives of an appropriate potential function, and thus they agree conceptually with the metric considered by Ruppeiner.[2] Therefore the metric geometry of thermodynamics based on (2.14) may be interpreted in terms of the thermodynamical fluctuation theory.[8,13] It is also important that g_{ij}, given by (2.14), have good properties with respect to the Legendre or, more generally, with respect to the contact transformations.[6] A glance at (2.1) and (2.3) or (2.14) makes it clear that the canonical distribution with its single stochastic variable $F_i=\mathcal{H}$—the Hamiltonian operator, and the only one statistical temperature $\beta^1=T^{-1}$ does not lead to the satisfactory geometrical picture. (Throughout this paper we set the Boltzmann constant k equal to 1.) The inner geometry of a one-dimensional manifold is trivial. One has therefore to take the grand canonical or the Boguslavski[14] distribution—or their counterparts for magnetic systems—for two-dimensional geometries, and their generalizations for higher dimensions.

III. CURVATURE OF THE PARAMETER SPACE

Our metric tensor (2.14) has a very special form because it is given by the matrix of second partial derivatives of the function $\ln Z$. Therefore one may expect that the formulas for the Christoffel symbols Γ_{ijk}, the curvature tensor R_{ijkl}, and the scalar curvature R will assume simplified forms. Indeed, the Christoffel symbols[15]

$$\Gamma_{ijk}=\tfrac{1}{2}(g_{ij,k}+g_{ik,j}-g_{jk,i}) \tag{3.1}$$

reduce in our case to

$$\Gamma_{ijk}=\tfrac{1}{2}g_{ij,k}=\tfrac{1}{2}f_{ijk}\ , \tag{3.2}$$

where for simplicity we have put

$$f=\ln Z\ ,\quad f_i=\frac{\partial \ln Z}{\partial \beta^i}\ ,\quad f_{ij}=\frac{\partial^2 \ln Z}{\partial \beta^i \partial \beta^j},\ldots\ . \tag{3.3}$$

As a consequence the curvature tensor is

$$R_{ijkl}=\tfrac{1}{2}(g_{jk,il}-g_{ik,jl}+g_{il,jk}-g_{jl,ik}) +g^{mn}(\Gamma_{mil}\Gamma_{njk}-\Gamma_{mik}\Gamma_{njl})\ , \tag{3.4}$$

and reduces to

$$R_{ijkl}=\tfrac{1}{4}g^{mn}(f_{mil}f_{njk}-f_{mik}f_{njl}) \tag{3.5}$$

because the fourth derivatives cancel each other.

In this paper we will consider only systems with two thermodynamical degrees of freedom. For a two-dimensional Riemann manifold there is only one independent nonvanishing component of the curvature tensor, namely, R_{1212}. Hence the scalar curvature

$$R=g^{mn}R^{i}_{nim} \tag{3.6}$$

simplifies to[15]

$$R=\frac{2}{g}R_{1212}\ ,\quad g=\det(g_{ij})\ . \tag{3.7}$$

It is interesting to note that R may be expressed by means of a determinant, namely,

$$R=\frac{-1}{2g^2}\begin{vmatrix} f_{11} & f_{12} & f_{22} \\ f_{111} & f_{112} & f_{122} \\ f_{112} & f_{122} & f_{222} \end{vmatrix}\ . \tag{3.8}$$

From (3.5) or (3.8), one can see that R is given in terms of the second and third derivatives of $\ln Z$. Physically, it means that R depends on the second and third moments of the variables F_i. Indeed, applying once more (2.10) to (2.12), one receives [cf. also (2.13)]

$$\frac{\partial^3 \ln Z}{\partial\beta^k\partial\beta^j\partial\beta^i}=-\int_0^1 d\lambda\,\mathrm{Tr}\left[\rho\left[\int_0^1 d\mu\, e^{-\mu A}(F_k-\langle F_k\rangle)e^{\mu A}e^{-\lambda A}(F_i-\langle F_i\rangle)e^{\lambda A}(F_j-\langle F_j\rangle) + \int_0^\lambda d\mu[e^{-\lambda A}(F_i-\langle F_i\rangle)e^{\lambda A}\ ,\ e^{-\mu A}(F_k-\langle F_k\rangle)e^{\mu A}](F_j-\langle F_j\rangle)\right]\right]\ , \tag{3.9}$$

where $A=-\beta^l F_1$ and [,] is the commutator. If F_i commute then this complicated expression reduces to

$$\frac{\partial^3 \ln Z}{\partial\beta^i\partial\beta^j\partial\beta^k}=-\langle(F_i-\langle F_i\rangle)(F_j-\langle F_j\rangle)(F_k-\langle F_k\rangle)\rangle\ . \tag{3.10}$$

That is why we name (3.9) the third moments of the quantum variables F_i.

IV. ONE-DIMENSIONAL ISING MODEL

A model of a magnetic system is typically composed of a set of N spins s_i, $i=1,2,\ldots,N$. We shall consider the simplest case when $s_i=+1$ or $s_i=-1$, corresponding to spin up or down, respectively. We shall also assume the S^1 topology of the spin chain, i.e., $s_{N+i}=s_i$. The Hamiltonian of the 1D Ising model is

$$\mathcal{H}=-J\sum_{k=1}^{N}s_k s_{k+1}-H\sum_{k=1}^{N}s_k\ , \tag{4.1}$$

where J is the coupling constant for the nearest-neighbor pairs in the lattice and H is the external magnetic field (multiplied by the magnetic dipole moment of one spin). $\mathcal{H}$ may be rewritten in the form

$$\mathcal{H}=F_1+F_2\ , \tag{4.2}$$

which indicates that we have two random variables: $F_1=-J\sum_k s_k s_{k+1}$ and $F_2=-H\sum_k s_k$. F_1 represents the interaction energy between spins, and, phenomenologically, it corresponds to the internal energy U, $F_1=U$. F_2 represents the interaction energy between the individual spins and the external field. Phenomenologically, F_2 corresponds to the global energy of interaction systems with external magnetic field $\langle F_2\rangle=-MH$; M is the magnetization of the chain. From this point of view the distribution function

$$\rho=Z^{-1}(\beta,\beta H)e^{-\beta\mathcal{H}}=Z^{-1}(\beta,\beta H)e^{-\beta F_1-\beta F_2}\ ,\quad \beta=T^{-1} \tag{4.3}$$

should not be treated as the canonical distribution, but rather as a magnetic counterpart of the Boguslavski distribution for gases. The reason is that for (4.3) $T\ln Z=-G$ (G is the Gibbs function) whereas for the canonical distribution one has $T\ln Z=-F$ (F is the free energy[14]). An extensive discussion of these problems can be found in the textbooks by Stanley,[16] Kittel,[17] Callen,[13] and many others.

For (4.1) in the limit of large N one obtains[18]

$$Z(\beta,\beta H)=e^{N\beta J}\{\cosh(\beta H)+[\cosh^2(\beta H)-2e^{-2\beta J}\sinh(2\beta J)]^{1/2}\}^N . \tag{4.4}$$

In order to simplify the notation and calculations we will use the abbreviations

$$x=\beta J,\quad y=\beta H,\quad A(x,y)=(e^{-4x}+\sinh^2 y)^{1/2} , \tag{4.5}$$

and then

$$f(x,y)=\frac{1}{N}\ln Z=x+\ln[\cosh y+A(x,y)] . \tag{4.6}$$

The components of the metric tensor we shall compute by means of $f(x,y)$, and therefore they will have an intensive character. According to the general rules developed in Sec. II, we have

$$\begin{aligned} g_{11}&=\frac{\partial^2 f}{\partial x^2}=A^{-3}(A+\cosh y)^{-2}[8A^2e^{-4x}(A+\cosh y)\\ &\qquad -4e^{-8x}(2A+\cosh y)] ,\\ g_{12}&=\frac{\partial^2 f}{\partial x\,\partial y}=2A^{-3}e^{-4x}\sinh y ,\\ g_{22}&=\frac{\partial^2 f}{\partial y^2}=A^{-3}e^{-4x}\cosh y , \end{aligned} \tag{4.7}$$

and

$$\det g=4A^{-4}e^{-8x}(\cosh y+A)^{-2} . \tag{4.8}$$

One can readily see that for $T\neq 0$, $H\to\infty$, all components $g_{ij}\to 0$, which means that all these fluctuations disappear (the magnetic saturation). However, for $H=0$, $T\to 0$, one has $g_{11}\to 0$, $g_{12}=0$, but $g_{22}\to\infty$ for $J>0$ and $g_{22}\to 0$ for $J<0$. The behavior of g_{22} for ferromagnetics, in this case, reflects the fact that the magnetic susceptibility χ_T tends to plus infinity in that limit.

We are working here in the coordinates x,y, i.e., in the coordinates T and H. Ruppeiner[19] used another system of coordinates, namely, T and M. His metric was diagonal and seemed to be much simpler than (4.7). However, the component $g_{TT}=T^{-1}(\partial S/\partial T)_M=T^{-2}c_M(T,M)$ involved the specific heat, which is such a complicated function of T and M that he was unable to perform all the calculations analytically. Therefore, he was forced to perform numerical computer calculations. With our metric tensor (4.7), though it is not diagonal, we are able to find the scalar curvature in a closed form. Of course, we do not have to calculate the fourth partial derivatives of $\ln Z$ because they cancel each other (cf. Sec. III). The third derivatives of $f(x,y)$ have the form

$$\begin{aligned} \frac{\partial^3 f}{\partial x^3}&=8A^{-5}e^{-4x}(A+\cosh y)^{-3}\left[-4A^4(A+\cosh y)^2+3e^{-4x}(A+\cosh y)(2A+\cosh y)(2A^2-e^{-4x})-2A^2e^{-8x}\right] ,\\ \frac{\partial^3 f}{\partial x^2\partial y}&=-8A^{-3}e^{-4x}\sinh y+12A^{-5}e^{-8x}\sinh y ,\\ \frac{\partial^3 f}{\partial x\,\partial y^2}&=A^{-5}e^{-4x}\cosh y(6e^{-4x}-4A^2) ,\\ \frac{\partial^3 f}{\partial y^3}&=A^{-5}e^{-4x}\sinh y(A^2-3\cosh^2 y) . \end{aligned} \tag{4.9}$$

Due to (4.7)–(4.9) and (3.8), after rather lengthy and tedious computations, we have received an amazingly simple expression for the scalar curvature R,

$$R=A^{-1}\cosh y+1=\cosh y(\sinh^2 y+e^{-4x})^{-1/2}+1 . \tag{4.10}$$

R is a positive function of x and y. Moreover, it is a symmetric function of y, and this means that the scalar curvature is independent of the orientation of the external magnetic field, $R(-H)=R(H)$. On the other hand, R behaves differently for positive x ($J>0$, ferromagnetism) and negative x ($J<0$, antiferromagnetism). For finite T and $H\to\infty$, we have $R\to\coth y+1=2$, whereas for finite T but $H\to 0$, we have $R\to e^{2x}+1=e^{2J/T}+1$. In Figs. 1 and 2 we present the dependence of R on H for a fixed value of T (for $J>0$ and $J<0$, respectively).

More interesting is the dependence of R on T. For $H=0$ and $T=0$, one has $R=e^{2x}+1=e^{2J/T}+1$. Further, in the limit $T\to\infty$, one has $R\to 2$ independently of the sign of J. On the other hand, if $T\to 0$, then $R\to+\infty$ for $J>0$ and $R\to 1$ for $J<0$. Figures 3 and 4 depict qualitatively the dependence of R on T. Similar behavior of R was found numerically by Ruppeiner.[19]

From (4.10) we see that $R\to 2$ for $J\to 0$. Therefore $R-2$ may be treated as a joint measure of fluctuations caused by mutual interaction of spins. In other words, $R-2$ is a measure of deviation of the system from ideal

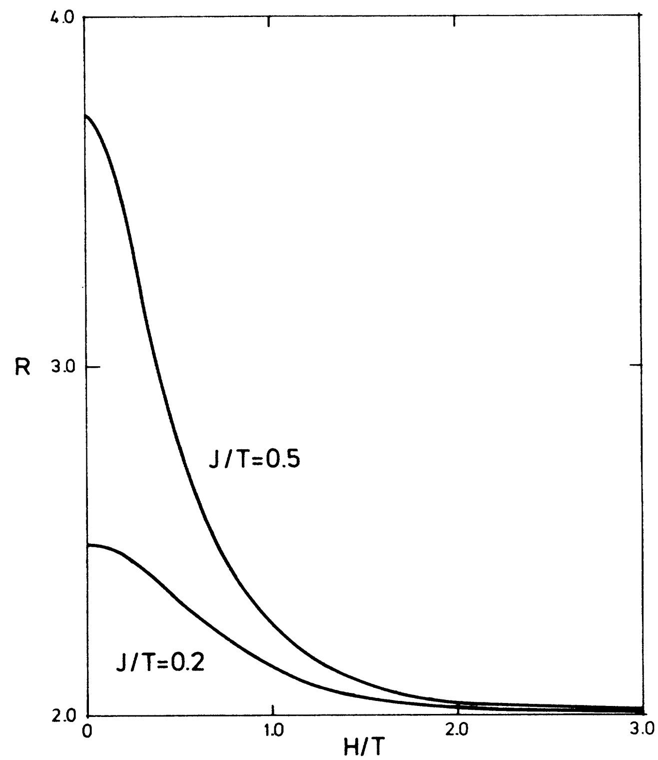

FIG. 1. Dependence of curvature R on magnetic field H by constant temperature T. Ferromagnetic case.

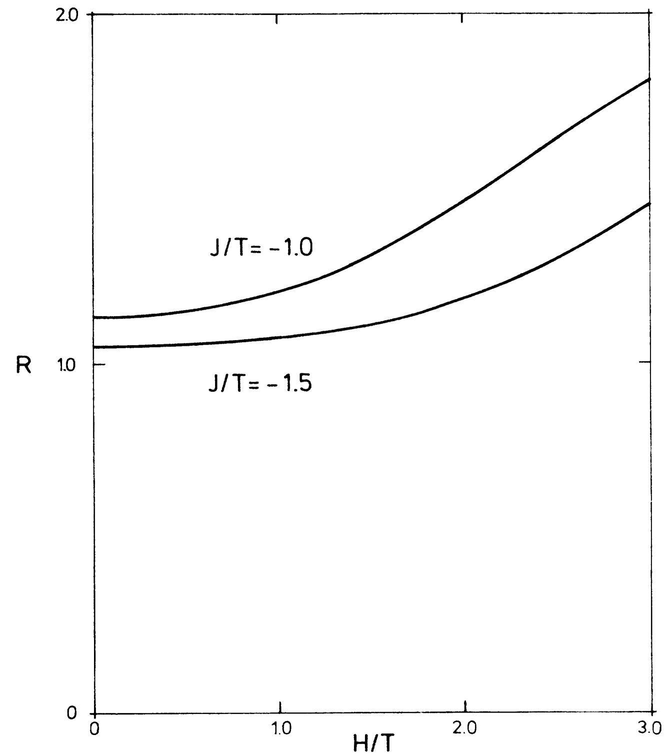

FIG. 2. Dependence of curvature R on magnetic field H by constant temperature T. Antiferromagnetic case.

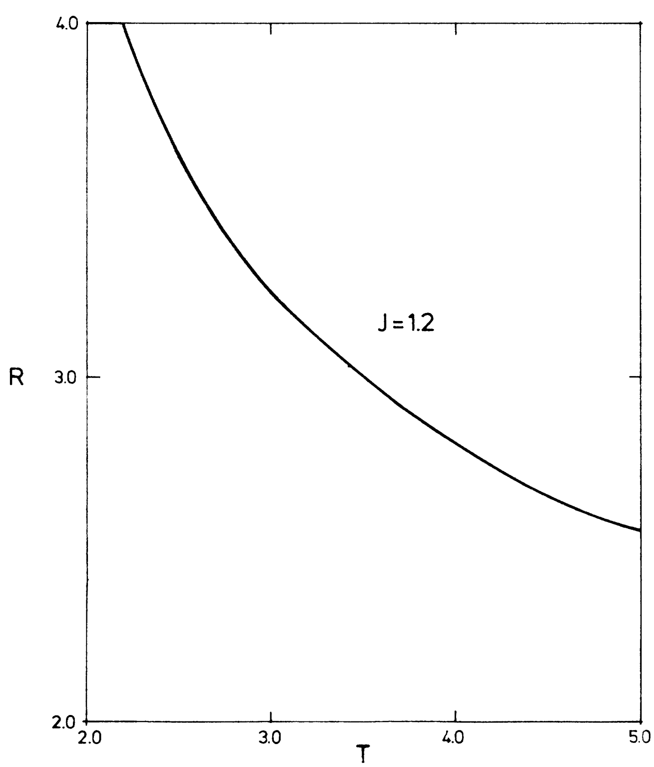

FIG. 3. Dependence of curvature R on temperature T by $H=0$. Ferromagnetic case.

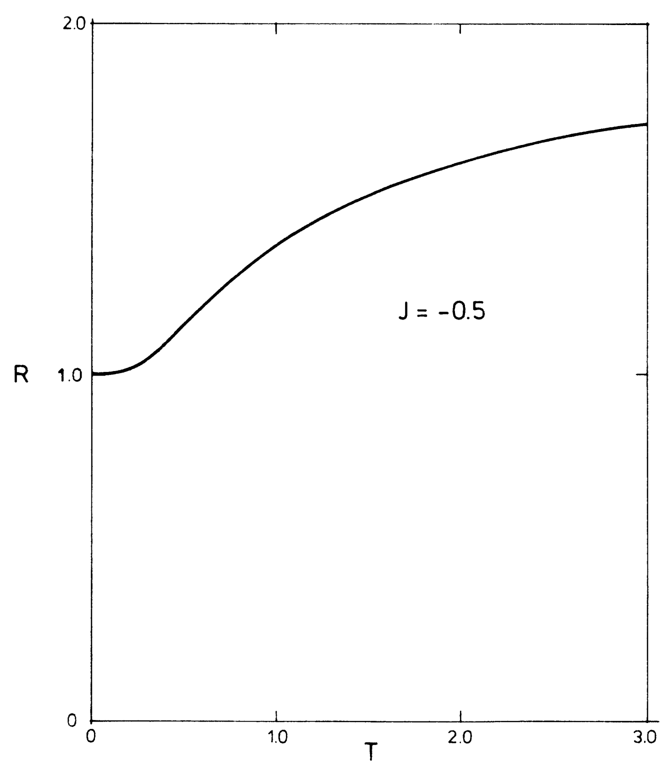

FIG. 4. Dependence of curvature R on temperature T by $H=0$. Antiferromagnetic case.

paramagnetism for which $J=0$.

The behavior of a system in the vicinity of the critical point is characterized mainly by the fluctuations of magnetization which is, in our case, given by $g_{22}=\langle(\sum_i s_i-\langle\sum_i s_i\rangle)^2\rangle$. Phenomenologically, it is connected with the magnetic susceptibility $\chi_T=T^{-2}g_{22}$. For $H=0$, g_{22} reduces to $g_{22}=e^{2x}=e^{2J/T}$. For the (1D) Ising model of ferromagnetics, the critical point is $H_c=0$, $T_c=0$. If $H=0$ and $T\to 0$, then $g_{22}\to+\infty$. Also for $T=$const and for increasing J, g_{22} increases.

For antiferromagnetics ($J<0$), $g_{22}=\exp(-2|J|/T)$ and an increase of $|J|$ causes a decrease of g_{22}. However, g_{22} is connected with the behavior of the correlation function[16] and not only with the correlation length, and at some point may be viewed as a measure of the stability of a system. Any description of a system by means of g_{22} or χ_T is far from being complete because it does not take into account fluctuations of energy in the system. The scalar curvature R takes into account all the relevant fluctuations, and R^{-1} may be taken as a new joint measure of the thermodynamical stability. One can readily see that for ferromagnetics any increase of J is accompanied by an appropriate increase of R, and the system becomes less stable. For antiferromagnetics, R decreases with increasing $|J|$ and the stability increases. Our results are in agreement with the result obtained by Ruppeiner. The interpretation of R as the quantity proportional to the correlation length seems to be much too strong. In the case of antiferromagnetics, R does not give the range of the envelope of the correlation function. In our paper we treat R as a new quantity describing the thermodynamical system, especially nearby critical points. Besides correlation length, correlation function, and isothermical susceptibility, R describes also the behavior of thermodynamical system. R is expressed not only by the second momenta, but also depends on the third momenta.

V. MEAN-FIELD METHOD

The phenomenological theory of ferromagnetism proposed by Weiss[16,20] is based on the assumption that the interaction of spins can be described by means of a mean molecular field which is proportional to the magnetization M. The essence of this assumption is that each spin interacts effectively with a mean field produced by all the other spins. It also means that the range of interaction is very long, and in fact each spin has an effective constant interaction with all the other spins (the situation is therefore opposite to that described by the Ising model). Such microscopic interpretation of the phenomenological theory of Weiss resulted because of Kac,[21] who considered a one-dimensional case, and Lebowitz and Penrose,[22] who generalized the results of Kac to higher dimensions.

Let us start therefore from the Hamiltonian

$$\mathcal{H}=\sum_{\substack{i,j\\1\le i<j\le N}}\Phi(|\mathbf{r}_i-\mathbf{r}_j|)s_is_j-H\sum_{i=1}^{N}s_i\ . \tag{5.1}$$

If each spin interacts with the same strength with all other spins, we may put[20]

$$\sum_{\substack{i,j\\1\le i<j\le N}}\Phi(|\mathbf{r}_i-\mathbf{r}_j|)s_is_j=-\frac{\alpha}{N}\sum_{\substack{i,j\\1\le i\le j\le N}}s_is_j\ , \tag{5.2}$$

where

$$\alpha=-\int\Phi(|\mathbf{r}|)d\mathbf{r}\ge 0\ . \tag{5.3}$$

Then $\mathcal{H}$ simplifies to

$$\mathcal{H}=-\frac{\alpha}{N}\sum_{\substack{i,j\\i<j}}s_is_j-H\sum_i s_i\ , \tag{5.4}$$

but it still has the structure $\mathcal{H}=F_1+F_2$, which is similar to (4.2). Therefore we have two stochastic variables

$$F_1=-\frac{\alpha}{N}\sum_{\substack{i,j\\i<j}}s_is_j\ ,\quad F_2=-H\sum_i s_i\ , \tag{5.5}$$

with the mean values

$$m_1=\langle F_1\rangle=U\ ,\quad m_2=\langle F_2\rangle=-HM\ . \tag{5.6}$$

The partition function for (5.4) can be written in the form

$$Z(\beta,\beta H)=\exp\left[-\frac{\alpha\beta}{2}\right]\sum_{\{s\}}\exp\left[\frac{\alpha\beta}{2N}\left[\sum_i s_i\right]^2+\beta H\sum_i s_i\right]\ , \tag{5.7}$$

where $\{s\}$ denotes a configuration of spins.

We shall, however, not need the explicit form of Z. Instead, we shall use some phenomenological formulas for components of the metric tensor. These components are expressed through thermodynamical response functions such as the heat capacities c_M and c_H and the magnetic susceptibility χ_T, which are known from (5.7), computed in the thermodynamical limit. The metric tensor, as it is defined by (2.14), is given in the coordinates $\beta^1=\beta=T^{-1}$ and $\beta^2=HT^{-1}$. We want to have it in the coordinates T and M. In our previous paper[6] we showed that

$$dl^2=g_{ij}d\beta^id\beta^j=g^{ij}dm_idm_j\ , \tag{5.8}$$

where

$$g^{ij}=-\frac{\partial^2 S}{\partial m_i\partial m_j} \tag{5.9}$$

(where S is the entropy) is inverse to $g_{ij}=\partial^2\ln Z/\partial\beta^i\partial\beta^j$, and m_i are given by (5.6). One may notice that (5.8) is the metric considered by Ruppeiner in his first paper[2] referring to the Riemannian geometry in thermodynamics. After two more transformations dl^2 may be rewritten in the form

$$\begin{aligned}dl^2&=-\frac{1}{T}\frac{\partial^2 U}{\partial\tilde{m}_i\partial\tilde{m}_j}d\tilde{m}_id\tilde{m}_j\\&=-\frac{1}{T}\frac{\partial^2 F}{\partial T^2}(dT)^2+\frac{1}{T}\frac{\partial^2 F}{\partial M^2}(dM)^2\ ,\end{aligned} \tag{5.10}$$

where $\tilde{m}_1=S$, $\tilde{m}_2=M$, and F is the free energy. The first equality of (5.10) has been received after a conformal transformation[6] from (5.9) and the second after subsequent Legendre transformation. Thus the metric tensor in the coordinates T and M is diagonal. Its components have very simple thermodynamic interpretation given by the following formulas:

$$g_{TT}=-\frac{1}{T}\left[\frac{\partial^2 F}{\partial T^2}\right]_M = c_M T^{-2} ,$$
$$g_{MM}=\frac{1}{T}\left[\frac{\partial^2 F}{\partial M^2}\right]_T = T^{-1}\chi_T^{-1} . \tag{5.11}$$

For the diagonal metric tensor (5.11) the scalar curvature R reduces to

$$R=-\frac{1}{\sqrt{g}}\left[\frac{\partial}{\partial T}\left[\frac{1}{\sqrt{g}}\frac{\partial g_{MM}}{\partial T}\right]+\frac{\partial}{\partial M}\left[\frac{1}{\sqrt{g}}\frac{\partial g_{TT}}{\partial M}\right]\right] . \tag{5.12}$$

R may also be rewritten in appropriately adapted form (3.8), namely, as

$$R=-\frac{1}{2g^2}\begin{vmatrix} -\frac{1}{T}\frac{\partial^2 F}{\partial T^2} & 0 & \frac{1}{T}\frac{\partial^2 F}{\partial M^2} \\ \frac{\partial}{\partial T}\left[\frac{1}{T}\frac{\partial^2 F}{\partial T^2}\right] & \frac{\partial}{\partial T}\left[\frac{1}{T}\frac{\partial^2 F}{\partial T \partial M}\right] & \frac{\partial}{\partial T}\left[\frac{1}{T}\frac{\partial^2 F}{\partial M^2}\right] \\ \frac{\partial}{\partial M}\left[\frac{1}{T}\frac{\partial^2 F}{\partial T^2}\right] & \frac{\partial}{\partial M}\left[\frac{1}{T}\frac{\partial^2 F}{\partial T \partial M}\right] & \frac{\partial}{\partial M}\left[\frac{1}{T}\frac{\partial^2 F}{\partial M^2}\right] \end{vmatrix} . \tag{5.13}$$

It is, however, well known that in the mean-field model the specific heat c_M becomes 0, $c_M=0$ (cf. Appendix). Hence $g_{TT}=0$ and $g=g_{TT}g_{MM}=0$, i.e., metric (5.11) degenerates in that model. This degeneration is caused by a constant interaction between arbitrary two spins. If we rewrite (5.4) in the form

$$\mathcal{H}=-\frac{\alpha}{2N}\sum_{i=1}^{N} s_i \sum_{j=1}^{N}{}' s_j - H\sum_{i=1}^{N} s_i , \tag{5.14}$$

where the prime indicates that $j\neq i$, and if we put

$$-\frac{\alpha}{2N}\sum_{j=1}^{N}{}' s_j = H_{\text{mol}} , \tag{5.15}$$

then $\mathcal{H}$ reduces to

$$\mathcal{H}=-(H_{\text{mol}}+H)\sum_i s_i = -H_{\text{eff}}\sum_i s_i . \tag{5.16}$$

H_{mol} and H_{eff} denote the mean-magnetic field produced by all spins but one, and the effective magnetic field $H_{\text{eff}}=H_{\text{mol}}+H$, respectively. As a matter of fact, the mean-field method is based on two assumptions, (5.2) and (5.15). The second of these replaces a stochastic variable

$$\sum_{j=1}^{N}{}' s_j$$

by its mean value $\sim H_{\text{mol}}$. As a result the Hamiltonian $\mathcal{H}$ has lost its structure F_1+F_2 because two linearly independent stochastic variables F_1 and F_2 have become linearly dependent due to (5.15). The new structure of (5.16) is $\mathcal{H}=H_{\text{eff}}F$. Consequently, we have only one statistical temperature βH_{eff} in the distribution function and the Riemannian structure has been lost.

In order to regain a Riemannian structure of the parameter space, we modify the Hamiltonian (5.4) by adding an additional term $\mathcal{H}_l$ corresponding to the mechanical energy of the spin lattice, i.e.,

$$\mathcal{H}=\mathcal{H}_l+\mathcal{H}_m , \tag{5.17}$$

where $\mathcal{H}_m$ is the magnetic Hamiltonian (5.4). Then g_{TT} is no longer zero, but we have

$$g_{TT}=c(T)T^{-2} , \quad g_{MM}=T^{-1}\chi_T^{-1} , \tag{5.18}$$

where $c(T)$ is the specific heat of the lattice. Because g_{TT} does not depend on M, the scalar curvature (5.12) reduces to

$$R=-\frac{1}{\sqrt{g}}\frac{\partial}{\partial T}\left[\frac{1}{\sqrt{g}}\frac{\partial g_{MM}}{\partial T}\right] . \tag{5.19}$$

We shall evaluate R in the vicinity of the critical Curie point. From (A16) in the Appendix we have

$$g_{MM}=T^{-1}\chi_T^{-1}=\frac{\epsilon}{\tilde{T}}+\eta^2 , \tag{5.20}$$

where $\epsilon=(T-T_c)/T_c$, $T_c=\alpha$ is the critical temperature[20] and $T=T/T_c$. Moreover, from (A16), we have for $\tilde{T}\rightarrow T_c$. Rewriting R in the form

$$R=\frac{\frac{\partial g}{\partial T}\frac{\partial g_{MM}}{\partial T}-2g\frac{\partial^2 g_{MM}}{\partial T^2}}{2g^2} \tag{5.21}$$

and taking into account that $g_{MM}\rightarrow 0$, $g\rightarrow 0$ but $\partial g_{MM}/\partial T\neq 0$ for $T\rightarrow T_c$, we see that the only nonvanishing term in the numerator is equal to $g_{TT}(\partial g_{MM}/\partial T)^2$. Therefore, for $T\to T_c$, one has

$$R=\frac{c(T)}{T^2}\frac{\left[\frac{\partial g_{MM}}{\partial T}\right]^2}{2g^2}\ , \tag{5.22}$$

and it is obvious that

$$R\to+\infty\ ,\quad \text{for } T\to T_c\ , \tag{5.23}$$

i.e., for the system approaching the critical point. As one can see from (5.21), the behavior of R for $T\to T_c$ does not depend on the unknown lattice specific heat $c(T)$.

Analogous calculations have been done for the van der Waals model of a real gas described by the Boguslavski or grand canonical distributions (results will be published later). It has turned out that all formulas are qualitatively identical with those given in this section, if one makes the obvious changes $c(T)\to c_V$, $g_{MM}\to g_{VV}$, and so on.

VI. CONCLUDING REMARKS

The scalar curvature R is a new function of the thermodynamic parameters not used in conventional thermodynamics. Although it can be found on a purely phenomenological level, the interpretation of R is connected with the statistical approach. More precisely, R is a function of the second and third moments of these stochastic variables which occur in the density operator ρ.

The results of this and our previous paper indicate some regularities in the behavior of R. First of all, R was always positive with only one exception, namely, that of the ideal fermionic gas for which R was negative. For the ideal classical gas, R was zero, and in the limit of the ideal paramagnetic, R was equal to 2. Thus R and $R-2$ measure deviations from the ideality of these two systems, respectively. Another point of interest is that R tended to plus infinity at the critical points. This allowed us to interpret R^{-1} as a new measure of the stability of the system. Typically, the criteria of stability are expressed through the second derivatives of thermodynamic potentials or (statistically) through the second moments of stochastic variables. Here R is a function of the second and third moments and hence R^{-1} is a measure of stability of higher order. The interpretation of R as the quantity proportional to the correlation length is too hasty. For near critical points for a gas or for a magnetic material this interpretation is, however, correct. We treat R as a quite new quantity describing the stability of the thermodynamical system. The correlation length is connected with second moments of correlations; R depends also on third moments.

It seems that R has a deeper meaning because of its relation with statistics and geometry. The scalar curvature R is the quantity constructed from tensor quantities. The geometrical analysis of thermodynamical systems gives deeper insight into the mathematical structure of statistical mechanics. We hope that R may be used as a verifying test for various statistical models. This means that only those models for which R behaves similarly to the considered standard models may be accepted. The open question is the phenomenological interpretation of R.

APPENDIX

In this appendix we want to show that $c_M=0$ for a system with Hamiltonian (5.4), i.e., in the mean field model. For that we have to calculate the free energy F of the system. Using the identity

$$e^{a/2}=(2\pi)^{-1/2}\int_{-\infty}^{+\infty}e^{-y^2/2+\sqrt{a}y}dy\ , \tag{A1}$$

we may rewrite (5.7) as

$$Z(N,T,H)=e^{-\nu/2}2^N\left[\frac{\nu N}{2\pi}\right]^{1/2}\int_{-\infty}^{+\infty}[e^{-\nu\eta^2/2}\cosh(\nu\eta+B)]^N d\eta\ , \tag{A2}$$

where $\nu=\alpha\beta$, $\eta=y(\nu N)^{-1/2}$, and $B=\beta H$ (for details see Thompson[20], Secs. 4 and 5). The integral in (A2) is of the form

$$I(N)=\int_{-\infty}^{+\infty}e^{n+(\eta)}d\eta\ , \tag{A3}$$

with

$$f(\eta)=-\frac{\nu\eta^2}{2}+\ln\cosh(\nu\eta+B)\ , \tag{A4}$$

and in the thermodynamic limit, $N\to\infty$ can be evaluated by the Laplace method. As a result we receive

$$-\frac{G}{T}=\lim_{N\to\infty}N^{-1}Z(N,T,H)=\ln 2+\max f(\eta)\ ,\qquad -\infty<\eta<+\infty \tag{A5}$$

where G is the Gibbs function per spin. The maximum of $f(\eta)$ is determined by

$$\eta=\tanh(\nu\eta+B)\ . \tag{A6}$$

The magnetization per spin $m(T,H)$ in the thermodynamic limit is given by

$$m(T,H)=\lim_{N\to\infty}N^{-1}M(T,H)=-\frac{\partial}{\partial B}\left[\frac{G}{T}\right]=\eta\ , \tag{A7}$$

where η is the solution of (A6), which maximizes $f(\eta)$. Thus η is interpreted as the magnetization per spin. The free energy per spin F is therefore given by the Legendre transform

$$F(T,\eta)=G(T,H(\eta))+\eta H(T,\eta)\ . \tag{A8}$$

Due to (A4) and (A5), we have

$$G=-T\ln 2+\frac{\alpha\eta^2}{2}-T\ln\cosh(\nu\eta+B)\ , \tag{A9}$$

where η fulfills (A6). From (A6) we have

$$\nu\eta+B=\operatorname{arctanh}\eta\ , \tag{A10}$$

and hence

$$G(T,\eta)=-T\ln 2+\frac{\alpha\eta^2}{2}+\frac{T}{2}\ln(1-\eta^2)\ . \quad \text{(A11)}$$

Moreover, from (A10) we have

$$H=T\,\text{arctanh}\eta-\alpha\eta\ , \quad \text{(A12)}$$

and, finally,

$$F(T,\eta)=-T\ln 2-\frac{\alpha\eta^2}{2}+\frac{T}{2}\ln(1-\eta^2)+T\eta\,\text{arctanh}\eta\ . \quad \text{(A13)}$$

$F(T,\eta)$ is a linear function of T, and so

$$c_M=-T\left[\frac{\partial^2 F}{\partial T^2}\right]_\eta=0\ . \quad \text{(A14)}$$

We are also interested in the magnetic susceptibility χ_T. From (A6) we have

$$\chi_T=\left[\frac{\partial\eta}{\partial H}\right]_T=\beta(1-\eta^2)[1-\nu(1-\eta^2)]^{-1}\ , \quad \text{(A15)}$$

and in the vicinity of the critical point, (A15) gives approximately

$$\chi_T^{-1}=\beta^{-1}(1+\eta^2)-\alpha\ . \quad \text{(A16)}$$

[1]F. Weinhold, J. Chem. Phys. **63**, 2479 (1975); **63**, 2484 (1975); **63**, 2488 (1975); **63**, 2496 (1975); **65**, 559 (1976).

[2]G. Ruppeiner, Phys. Rev. A **20**, 1608 (1979).

[3]R. Gilmore, Phys. Rev. A **30**, 1994 (1984).

[4]B. Andresen, R. S. Berry, R. Gilmore, E. Ihring, and P. Salamon (unpublished).

[5]H. Janyszek, Rep. Math. Phys. **24**, 1 (1986); **24**, 11 (1986).

[6]H. Janyszek and R. Mrugała, Rep. Math. Phys. (to be published).

[7]H. Janyszek and R. Murgała, J. Phys. (to be published).

[8]W. K. Wootters, Phys. Rev. D **23**, 357 (1981).

[9]L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, New York, 1977).

[10]R. S. Ingarden, H. Janyszek, A. Kossakowski, and T. Kawaguchi, Tensor N.S. **37**, 105 (1982).

[11]H. Umegaki, Kodai Math. Semin. Rep. **14**, 59 (1962).

[12]R. M. Wilcox, J. Math. Phys. **4**, 884 (1967).

[13]H. B. Callen, *Thermodynamics* (Wiley, New York, 1960).

[14]R. Kubo, *Statistical Mechanics* (North-Holland, Amsterdam, 1965); the Boguslavski distribution is more often referred to as the *P-T* distribution.

[15]B. A. Dubrowvin, A. T. Fomenko, and S. P. Nivikov, *Modern Geometry* (Springer, New York, 1984).

[16]H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Clarendon, Oxford, 1971).

[17]Ch. Kittel, *Elementary Statistical Physics* (Wiley, New York, 1958).

[18]K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).

[19]G. Ruppeiner, Phys. Rev. A **24**, 488 (1981).

[20]C. J. Thompson, *Mathematical Statistical Mechanics* (Princeton University Press, Princeton, NJ, 1972).

[21]M. Kac, *Mathematical Mechanisms Of Phase Transitions* (Gordon and Breach, New York, 1968).

[22]J. Lebowitz and O. Penrose, J. Math. Phys. **7**, 98 (1966).