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Asymptotic Forms for Correlation Functions*

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The range of validity of a general argument for the asymptotic form of correlation functions, presented in a previous paper, is discussed in some detail. The asymptotic form of correlation functions of local variables for one-dimensional lattice and continuous systems are discussed and found to have the predicted form.

I. INTRODUCTION

In a previous paper[1] (hereafter I) a plausible general argument was given for a certain asymptotic form for the correlation function of two local dynamical variables. It was argued that if $A(\vec{r})$ and $B(\vec{r})$ are local dynamical variables and ω stands for the variables specifying the thermodynamic state of the system then for ω near the critical point ω_c and r large enough

$$\langle A(\vec{r})B(0)\rangle - \langle A(\vec{r})\rangle\langle B(0)\rangle \simeq d_A(\omega)d_B(\omega)e^{-\kappa(\omega)r}/r^{b(\omega)}, \tag{1-1}$$

where $\langle\cdots\rangle$ is the usual average over an equilibrium ensemble. The functions $\kappa(\omega)$ and $b(\omega)$ are the same for a large class of A and B and $\kappa(\omega)\to 0, b(\omega)\to b \geqslant 0$ as $\omega\to\omega_c$. Near the critical point and for external field equal to zero the spin-spin, spin-energy density and energy-density-energy-density correlation functions of the two dimensional square spin-$\frac{1}{2}$ Ising model are known[2] and have been shown[1] to satisfy Eq. (1-1) for $T<T_c$ (the critical temperature). One might still argue that (1-1) is not a general property of systems in thermal equilibrium, but rather depends on some special properties of the example given. In particular it might depend on: (a) the system being two dimensional, (b) the nearest-neighbor interaction, (c) the system being spin $\frac{1}{2}$, (d) the fact that the external field was zero, (e) the particular choices of dynamical variables $A(\vec{r})$ and $B(\vec{r})$, and (f) the system being a lattice rather than a continuous system. Points (d) and (e) fall under the general question: For what class of variables $A(\vec{r})$, $B(\vec{r})$ and what thermodynamic states ω is (1-1) true? This question is discussed in general in Sec. II.

In Sec. III we discuss the asymptotic form of the correlation function for any two local variables of a one-dimensional Ising model for arbitrary spin and any finite range interaction and for any equilibrium state. We find that (1-1) is satisfied except for certain apparently rather unusual cases. These examples are pertinent to all of the above mentioned questions except (f). We also consider the correlation functions of a one-dimensional gas with nearest-neighbor interactions, and find that this continuous system has similar properties.

II. GENERAL DISCUSSION

We shall use the notation

$$C(A,B;r,\omega) = \langle A(\vec{r})B(0)\rangle - \langle A(\vec{r})\rangle\langle B(0)\rangle, \qquad (2\text{-}1)$$

sometimes suppressing an argument when of no interest. We shall assume, for simplicity, that (2-1) is a function of only the magnitude of $\vec{r}$ and that $C(A,B;\ r,\omega) = C(B,A;\ r,\omega)$. In I it was argued that for r large enough

$$C(A,B;r,\omega) = d_A(\omega)d_B(\omega)f(r,\omega), \qquad (2\text{-}2)$$

where $f(r,\omega)$ is the same function for essentially all local dynamical variables A and B. A somewhat extended version of the argument gave

$$f(r,\omega) = e^{-\kappa(\omega)r}/r^{b(\omega)},$$

which, with (2-2) yields (1-1).

We want to discuss ways in which (2-2) might fail. One way that (2-2) can fail is if we can find two different correlation functions for which the function $f(r,\omega)$ is different. We shall show that this must always be possible. Suppose we have two correlation functions $C(A,A)$ and $C(A,B)$ for which (2-2) holds. We can construct one for which (2-2) is false. Presumably (2-2) is the first term in an asymptotic expansion of the correlation functions, so let us write for r large

$$C(A,A;r,\omega) \simeq d_A^{\,2}(\omega)f(r,\omega) + g_{AA}(r,\omega), \qquad (2\text{-}3)$$

$$C(A,B;r,\omega) \simeq d_A(\omega)d_B(\omega)f(r,\omega) + g_{AB}(r,\omega), \qquad (2\text{-}4)$$

where the g functions are small compared to f for large r. The assumption that (2-2) is true for these correlations is equivalent to requiring $d_A(\omega) \neq 0$ and $d_B(\omega) \neq 0$ in (2-3) and (2-4). Now if $A(\vec{r})$ and $B(\vec{r})$ are local dynamical variables and a and b are constants, then $D(\vec{r}) = aA(\vec{r}) + bB(\vec{r})$ is another local dynamical variable. It is trivial that

$$C(A,D;r,\omega) = aC(A,A;r,\omega) + bC(A,B;r,\omega), \qquad (2\text{-}5)$$

Hence from (2-3), (2-4), and (2-5) we have, for r large

$$C(A,D;r,\omega) \simeq d_A(\omega)d_D(\omega)f(r,\omega) + ag_{AA}(r,\omega) + bg_{AB}(r,\omega), \qquad (2\text{-}6)$$

where $d_D(\omega) = ad_A(\omega) + bd_B(\omega)$. (2-7)

One can choose a and b so that $d_D(\omega) = 0$ for some fixed ω, hence $C(A,D)$ will vanish more rapidly for large r than $f(r,\omega)$ by virtue of (2-6). Furthermore, the correlation of D with any other dynamical variable will vanish faster than $f(r,\omega)$. For fixed $D(\vec{r})$, or equivalently fixed a and b, at what points ω can we expect the (hopefully) anamolous behavior $d_D(\omega) = 0$? Suppose ω stands for two thermodynamic variables. Then if $d_A(\omega) \neq 0$ and $d_B(\omega) \neq 0$, we would expect the solutions of $d_D(\omega) = 0$, if any, to form a line of points in the ω plane, but in general we would not expect the solutions to form a two-dimensional manifold. This leads one to conjecture that the proposed asymptotic form (2-2) is valid for any pair of local dynamical variables, $A(\vec{r})$ and $B(\vec{r})$, for any thermodynamic state ω, except for at most two lines in the ω plane (one associated with each dynamical variable) which are the points, if any, where $d_A(\omega) = 0$ or $d_B(\omega) = 0$. We shall see that this conjecture seems to be true for the one-dimensional models to be considered. We shall call the set of points for which $d_A(\omega) = 0$ the zero line of A.

For the two-dimensional Ising models it is known[2,3] that above the critical temperature and in zero field, the energy-density-correlation function vanishes faster with r than the spin-spin correlation function. The spin-energy-density correlation function is zero. We suppose that this is the line of zeros of the energy density. To verify this supposition we would have to show that all three correlations have the same asymptotic dependence for $T > T_c$ but non-zero external field. Unfortunately, the correlation functions are not known there. We shall see that there is a similar behavior in the one-dimensional Ising models where these conjectures can be verified.

Another way that (2-2) can fail, even if the function multiplying $f(r,\omega)$ is not zero, is for this function of ω not to have the product form $d_A(\omega)d_B(\omega)$. It is difficult to say anything in general but we shall investigate this possibility for the one-dimensional Ising model.

III. ONE-DIMENSIONAL MODELS

We now consider the correlation functions for some one-dimensional models. We take first the Ising chain of any spin and finite range of interaction. We have found that the form (1-1) follows rather directly from the existence of a transfer matrix formalism.

Consider an Ising chain where each site interacts with its γ nearest neighbors and which is $n\gamma$ sites long. Suppose the spin variable on each site varies from S to $-S$ in integer steps, where S is integer or half-integer. All of the equilibrium properties of such a system can be expressed in terms of a $(2S+1)^{\gamma}$ dimensional transfer matrix by a straightforward extension of the techniques used in the nearest-neighbor spin-$\frac{1}{2}$ chain.[4-6] One can write the correlation function of two groups of spins, one group on the sites $i_1 < i_2 < \cdots < i_q$, and the other at $r\gamma + j_1 < r\gamma + j_2 < \cdots < r\gamma + j_p$, in the form

$$\langle i_1,\ldots,i_q,r\gamma+j_1,\ldots,r\gamma+j_p\rangle$$
$$-\langle i_1,\ldots,i_q\rangle\langle j_1,\ldots,j_p\rangle$$
$$=\sum_{\alpha>0}\underline{M}(i_1,\ldots,i_q)_{0\alpha}$$
$$+\underline{M}(j_1,\ldots,j_p)_{\alpha 0}(\lambda_\alpha/\lambda_0)^r, \tag{3-1}$$

where λ_0 is the largest eigenvalue of the transfer matrix (which can be shown to be nondegenerate) and α runs over the other eigenvalues. $\underline{M}(i_1,\ldots,i_q)$ is an operator depending only on the differences $i_1-i_2, i_2-i_3,\ldots$ and is taken in the basis diagonalizing[7] the transfer matrix. The correlation function of any two local variables can be written as a linear combination of the above type of functions. In order that the asymptotic form of (3-1) agree with (1-1) it is sufficient that the second-largest eigenvalue λ_1 of the transfer matrix be nondegenerate and that the matrix elements M_{01} and M_{10} be non-zero. The eigenvalues and the matrix elements are functions of the temperature T and the magnetic field B. The vanishing of the matrix elements on lines in the (T,B) plane is consistent with the discussion of Sec. II; however, they must not vanish over the whole (T,B) plane.

We have not been able to prove that the general Ising chain has the above two properties. On the other hand, we have not been able to find any particular model for which either property is missing. For the nearest-neighbor spin-$\frac{1}{2}$ model there are only two eigenvalues[6] and these are nondegenerate. In this case (3-1) has only one term and the form (1-1) is obtained even for small r. This is a special property of this model. One can verify that the matrix elements do not vanish identically by direct computation. For the nearest-neighbor spin-1 and spin-$\frac{3}{2}$ case the eigenvalues are known[8] for $B=0$ (and by perturbation theory for small B) and again neither λ_0 nor λ_1 is degenerate. Temperly[9] has solved the next-nearest-neighbor spin-$\frac{1}{2}$ model for $B=0$ and again λ_0 and λ_1 are nondegenerate. A direct calculation of the matrix elements would be algebraically complicated in these last two cases and has not been done. There is no reason to believe they are identically zero.

For the general Ising chain every element of the transfer matrix is positive and a theorem due to Perron says that λ_0 is nondegenerate for such matrices. Unfortunately there seems to be no applicable theorems concerning the degeneracy of λ_1. We can consider the general models in limited regions of the thermodynamic plane. Both high- and low-temperature expansion suggest themselves. In the low-temperature region $T\to 0$, $B=0$, for a ferromagnetic Ising chain, two of the diagonal matrix elements of the transfer matrix become large compared to all others. The transfer matrix $\underline{P}=\exp(c/kT)\underline{P}'$, where c is a constant and $\underline{P}'$ is a matrix whose elements all approach zero continuously as $T\to 0$ except for the first two on the diagonal which approach 1. In this limit the transfer matrix is diagonal and its two largest eigenvalues are degenerate with each other but not with any other eigenvalue. For T small enough, by continuity in T, these two eigenvalues must still be larger than any other. For T small but nonzero the transfer matrix has positive elements and therefore has a nondegenerate largest eigenvalue. Hence in the neighborhood of $T=0$ neither λ_0 nor λ_1 is degenerate and in fact

$$\lambda_1/\lambda_0\to 1,\quad \lambda_i/\lambda_0\to 0 \text{ for } i>1,$$
$$\lambda_0\to\infty \text{ as } T\to 0, \tag{3-2}$$

so that the non-degeneracy condition is satisfied for a rather large class of Ising chains in this limited region of the thermodynamic plane. For these models there is only one characteristic length appearing in the correlation functions at small T and this length goes to infinity as $T\to 0$. If we look at (3-1) for fixed r (not necessarily large) but as $T\to 0$ for $B=0$, the result (3-2) shows that only the λ_1/λ_0 term contributes, and since $\lambda_1/\lambda_0\to 1$ this term becomes very long ranged. Thus $T=0$, $B=0$ appears in some respects like a critical point; an observation often made in connection with the divergence of the susceptibility at this point.

For the general Ising chain and arbitrary B the transfer matrix approaches a matrix whose every element is 1 as $T\to\infty$. Call this matrix $\underline{U}$ and write the transfer matrix as $\underline{T}=\underline{U}+(\underline{T}-\underline{U})$, where $\underline{T}-\underline{U}\to 0$ as $T\to\infty$. The obvious thing to do is diagonalize $\underline{U}$ and treat $\underline{T}-\underline{U}$ by perturbation theory. $\underline{U}$ is a cyclic matrix and can be diagonalized by standard methods.[10] All of its eigenvalues are zero except one which is equal to the dimension of $\underline{U}$. Hence for $T\to\infty$, λ_0 is nondegenerate, but $\lambda_1=0$ and is degenerate with all the other eigenvalues. In this limit the correlation functions (3-1) vanish, as they should for high temperatures. To move slightly away from $T=\infty$ we can try to find the perturbation-theory corrections to the eigenvalues treating $(\underline{T}-\underline{U})$ as small. This is easy for λ_0 and produces a high-temperature expansion of the partition function. To find the asymptotic form of the correlation functions at high temperature we must find the corrections to λ_1. The transfer matrix has dimension $(2S+1)^\gamma$ and λ_1 is a $[(2S+1)^\gamma-1]$-fold degenerate eigenvalue in zero order. To do even first-order perturbation theory we must diagonalize a $(2S+1)^\gamma-1$ submatrix of $\underline{T}-\underline{U}$. For γ or S large this seems to be no easier then diagonalizing the whole transfer matrix itself. It is strange that going to high temperatures, which immensely simplifies the computation of the partition function, produces no similar simplification in the computation of the asymptotic form of the correlation functions.

We now consider a one-dimensional gas of particles interacting by a pair potential with the properties

$$\phi(r)=\infty \text{ for } r<a,\quad \phi(r)=0 \text{ for } r\geqslant 2a. \tag{3-3}$$

These conditions imply that only nearest neighbors can interact. The correlation function of any two physical local variables can be written as an integral or a sum of integrals of the reduced distribution functions

$$f_n(y_1,\dots,y_n) = \Big\langle \sum_{i_n=1}^{N} \cdots \sum_{i_1=1}^{N}{}' \times \delta(x_{i_1}-y_1)\cdots\delta(x_{i_n}-y_n)\Big\rangle, \quad (3\text{-}4)$$

where the prime on the sum means no two indices are the same and $x_1,\dots,x_N$ are the coordinates of the particles. One can also assume $y_1 < y_2 < y_3 \cdots < y_n$ because any configuration not satisfying this condition is a permutation of a configuration which does, and (3-4) is invariant under permutations of the $y_1,\dots,y_n$. In the thermodynamic limit, as the length of the gas and the number of particles go to infinity with the length per particle approaching L, the f_n become functions of only the differences $y_2-y_1,\dots,y_n-y_1$ by translational invariance. Salsburg, Zwanzig and Kirkwood[11] have computed the reduced distribution functions of this model. The result that we need from their work is that the reduced distribution functions obey, in the thermodynamic limit, the superposition principle

$$f_n(y_1,\dots,y_n) = L^{n-2} \prod_{i=1}^{n-1} f_2(y_{i+1}-y_i). \quad (3\text{-}5)$$

Let the coordinates $y_1,\dots,y_n$ split into two groups $y_1<y_2<\cdots<y_j$ and a second group we label $z_1<z_2<\cdots<z_k$, and measure the distance between the groups by $r=z_1-y_j$. We want to let r become large while keeping the distances

$$y_{21}=y_2-y_1,\dots,y_{j1}=y_j-y_1, \text{ and } z_{21} = z_2-z_1,\dots,z_{k1}=z_k-z_1$$

fixed. If we define

$$C_{j+k}(y_{21},\dots,y_{j1};z_{21},\dots,z_{k1};r) = f_{j+k}(y_1,\dots,z_k) - f_j(y_1,\dots,y_j) \times f_k(z_1,\dots,z_k),$$

then one can show from (3-5) that

$$C_{j+k}(y_{21},\dots,y_{j1};z_{21},\dots,z_{k1};r) = L^2 f_j(y_{21},\dots,y_{j1}) f_k(z_{21},\dots,z_{k1}) \times[f_2(r)-L^{-2}]. \quad (3\text{-}6)$$

Since $f_2(r)$ approaches L^{-2} for large r the correlation function vanishes as it should. For fixed $y_{21},\dots,z_{k1}$ this correlation function is of the form (2-2). One can show that these correlation functions have the slightly stronger form (1-1), but the computation is too detailed to present here. This result is a direct consequence of the principle of superposition, and it is easy to see the principle of superposition depends on the interaction being no more than nearest neighbor. To extend this calculation to longer-range forces appears to be rather complicated. One can formulate the problem, in analogy with the Ising models, in a transfer-operator manner and indeed Van Hove[12] has studied the thermodynamic properties of these models in this way. Unfortunately the structure of the correlation functions is not known.

The result (3-6), and the corresponding results for the Ising models, depend on defining the distance r between the groups of variables as the smallest distance between members of the groups. Local variables have some spatial extension so that the distance between two such variables is not, in general, uniquely defined and this is something of a difficulty with (2-2) unless one has a specific model where the definition of the distances is clear. Near the critical point, however, this difficulty disappears because the correlation functions become very long ranged and hence insensitive to the exact definition of the distance.

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