Decay of the direct correlation function in linear lattice systems

M. Robert
Baker Laboratory, Cornell University, Ithaca, New York 14853
(Received 2 September 1983)

The direct correlation function of the one-dimensional lattice-gas (Ising) model with nearest-neighbor and next-nearest-neighbor interactions is calculated exactly. It is shown that, depending on the strengths and signs of the coupling constants, the direct correlation function can either have a finite range equal to that of the interactions, or decay exponentially in a monotonic or oscillatory fashion. At the critical point, which occurs at zero temperature, the direct correlation function is found in all cases to have exactly the range of the interactions, while its values become unbounded; this is in contrast to earlier nonrigorous results. The second moment of the direct correlation function is found to diverge at the critical point, in the neighborhood of which it becomes proportional to the correlation length of the density (spin) fluctuations, confirming a prediction of scaling theory in one dimension.

I. INTRODUCTION

The direct correlation function, introduced by Ornstein and Zernike[1] in 1914 in their study of the scattering of light by fluids near their critical point plays a central role in the statistical mechanics of both uniform[2(a)] and nonuniform[2(b)] classical systems.

The motivation for introducing the direct correlation function was to describe the long-ranged density fluctuations of a near-critical fluid in terms of correlations which, like the molecular interactions themselves, would remain short ranged in the critical region.

Ornstein and Zernike originally assumed that at the critical point of a three-dimensional fluid the Fourier transform of the direct correlation function is analytic at the origin, which amounts to assuming that in real space, the direct correlation function is a bounded function which is either of finite range or decays exponentially.

That such a property of the direct correlation function cannot hold in general was established by the exact results for the pair correlation function of the two-dimensional lattice-gas (Ising) model with nearest-neighbor interactions,[3] which imply that at the critical point, the Fourier transform of the direct correlation function is not analytic at the origin, although the precise nature of the asymptotic decay in real space of the direct correlation function of that model is not known.

In a series of studies of one-dimensional lattice or continuum models with nearest-neighbor interactions,[4–7] Percus has shown that the direct correlation function has always exactly the range of the interactions. Similar exact results hold for the spherical model and the ideal Bose gas in any number of dimensions[8,9] and, as is well known, for the one-dimensional fluid of hard rods.[10] Their validity has recently been extended by Percus to Baxter's model of sticky hard rods.[6]

In this paper we study the decay properties of the direct correlation function of a somewhat more complex linear system, the one-dimensional lattice-gas (Ising) model with both nearest- and next-nearest-neighbor interactions.

In Sec. II, we present the results of the calculation of the pair correlation function of the model. In Sec. III, the expression of the pair correlation function obtained in Sec. II is used to calculate the direct correlation function. The decay properties of the direct correlation function are determined in Sec. IV in terms of the nearest- and next-nearest-neighbor interactions and of the temperature. In Sec. V, we analyze the critical behavior of the direct correlation function and that of its second moment. Section VI concludes this paper with a summary and a discussion of the results.

II. PAIR CORRELATION FUNCTION

It is straightforward, although lengthy, to calculate, using the transfer-matrix method, the exact expression of the pair correlation function of the one-dimensional lattice-gas (Ising) model with nearest- and next-nearest-neighbor interactions. Since this calculation had already been carried out by Stephenson,[11] we shall not present our detailed calculations but only quote the final result.

In the Ising transcription of the lattice gas we have spins ± 1 located at the lattice sites. We shall denote by J_1 and J_2 the interaction energies between a pair of nearest-neighbor spins and a pair of next-nearest-neighbor spins, respectively, and by $h(|n|)$ the pair correlation function between spins located at sites an integer distance $|n|$ [$n \in Z$, the set of all (positive and negative) integers, including 0] apart.

The interaction energy U_N for a configuration $\{s\}$ of N spins $s_1, \ldots, s_N$ is

$$U_N(\{s\}) = J_1 \sum_{i_1=1}^{N} s_i s_{i+1} + J_2 \sum_{i=1}^{N} s_i s_{i+2}$$

with periodic boundary conditions $s_{k+N} \equiv s_k$ for all k. The corresponding pair correlation function is

$$h_N(|n|) = \frac{\sum_{\{s\}} s_0 s_n e^{-U_N(\{s\})/k_B T}}{\sum_{\{s\}} e^{-U_N(\{s\})/k_B T}}, \quad n \neq 0$$

with k_B Boltzmann's constant and T the absolute temperature.

At the thermodynamic limit we find

$$h(|n|)=\lim_{N\to\infty} h_N(|n|) =\alpha e^{-\kappa_1|n|}+\beta e^{-\kappa_2|n|}, \quad |n|\neq 0 \tag{2.1}$$

with

$$\kappa_1=-\ln(\mu_+/\lambda), \quad \kappa_2=-\ln(\mu_-/\lambda), \quad \alpha=\tfrac{1}{2}(1+\epsilon), \tag{2.2}$$

and

$$\beta=\tfrac{1}{2}(1-\epsilon),$$

where, in terms of the dimensionless coupling constants $\mathscr{J}_1\equiv J_1/k_BT$ and $\mathscr{J}_2\equiv J_2/k_BT$,

$$\lambda=e^{\mathscr{J}_2}[\cosh\mathscr{J}_1+(\sinh^2\mathscr{J}_1+e^{-4\mathscr{J}_2})^{1/2}],$$
$$\mu_\pm=e^{\mathscr{J}_2}[\sinh\mathscr{J}_1\pm(\cosh^2\mathscr{J}_1-e^{-4\mathscr{J}_2})^{1/2}], \tag{2.3}$$

and

$$\epsilon=\frac{1}{2}\frac{\sinh(2\mathscr{J}_1)}{[(\sinh^2\mathscr{J}_1+e^{-4\mathscr{J}_2})(\cosh^2\mathscr{J}_1-e^{-4\mathscr{J}_2})]^{1/2}}.$$

III. DIRECT CORRELATION FUNCTION

The direct correlation function $c(|n|)$ is defined in terms of the pair correlation function $h(|n|)$ by the relation[2(a)]

$$h(|n|)=c(|n|)+\tfrac{1}{2}\sum_{n'\in Z} h(|n-n'|)c(|n'|). \tag{3.1}$$

Relation (3.1) is the discrete version of the more familiar Ornstein-Zernike relation appropriate to spatially uniform continuous systems:[1]

$$h(|r|)=c(|r|)+\rho\int h(|r-r'|)c(|r'|)dr',$$

where $|r|$ denotes the distance between two particles separated by the vector r and ρ is the average density. The factor $\frac{1}{2}$ appearing in the right-hand side of (3.1) is the density ρ of the lattice gas in the absence of an external field, in which a particle is present or absent in a given cell with an equal probability of $\frac{1}{2}$. Defining the discrete Fourier transforms

$$\hat{h}(q)=\sum_{n\in Z} h(|n|)e^{iqn}$$

and (3.2)

$$\hat{c}(q)=\sum_{n\in Z} c(|n|)e^{iqn},$$

relation (3.1) becomes

$$\hat{c}(q)=\frac{2\hat{h}(q)}{2+\hat{h}(q)}. \tag{3.3}$$

Using expression (2.1) for $h(|n|)$ gives for $\hat{h}(q)$

$$\hat{h}(q)=h(0)+\sum_{\substack{n\in Z\\ n\neq 0}} e^{iqn}(\alpha e^{-\kappa_1|n|}+\beta e^{-\kappa_2|n|}), \tag{3.4}$$

where the term $h(0)\equiv h(|0|)\equiv h(n=0)$ has been separated from the sum.

$h(|n|)$ is related to the distribution function $g(|n|)$ by $h(|n|)=g(|n|)-1$, and $g(n)$ is proportional to the probability of finding the spin at site n in a given state given that the spin at the origin is in that same state. But in the Ising model two spins cannot lie on the same lattice site, so that $g(0)=g(|0|)\equiv g(n=0)=0$ and therefore $h(0)=g(0)-1=-1$.

The sums in (3.4) are readily carried out with the result

$$\hat{h}(q)=-1+2\alpha\frac{e^{\kappa_1}\cos q-1}{e^{2\kappa_1}-2e^{\kappa_1}\cos q+1} +2\beta\frac{e^{\kappa_2}\cos q-1}{e^{2\kappa_2}-2e^{\kappa_2}\cos q+1}, \tag{3.5}$$

where we have used $h(0)=-1$.[12]

Inserting (3.5) into (3.3) gives

$$\hat{c}(q)=2\frac{a_1+b_1\cos q+c_1\cos^2 q}{a_2+b_2\cos q+c_2\cos^2 q} \tag{3.6}$$

with

$$\begin{aligned}
a_1&=-e^{2\kappa_1+2\kappa_2}-(1+2\beta)e^{2\kappa_1}-(1+2\alpha)e^{2\kappa_2}-1-2(\alpha+\beta),\\
b_1&=2(1+\alpha)e^{\kappa_1+2\kappa_2}+2(1+\beta)e^{2\kappa_1+\kappa_2}+2(1+\alpha+2\beta)e^{\kappa_1}+2(1+\beta+2\alpha)e^{\kappa_2},\\
c_1&=-4(1+\alpha+\beta)e^{\kappa_1+\kappa_2},\\
a_2&=e^{2\kappa_1+2\kappa_2}+(1-2\beta)e^{2\kappa_1}+(1-2\alpha)e^{2\kappa_2}-1,\\
b_2&=2(\alpha-1)e^{\kappa_1+2\kappa_2}+2(\beta-1)e^{2\kappa_1+\kappa_2}+2(\alpha+2\beta-1)e^{\kappa_1}+2(2\alpha+\beta-1)e^{\kappa_2},\\
c_2&=4(1-\alpha-\beta)e^{\kappa_1+\kappa_2}.
\end{aligned} \tag{3.7}$$

These expressions can be rewritten by using the fact that $\alpha=1-\beta$, which follows from (2.2). We find

$$\begin{aligned}
a_1&=-e^{2\kappa_1+2\kappa_2}-(1+2\beta)e^{2\kappa_1}-(3-2\beta)e^{2\kappa_2}-3,\\
b_1&=2(2-\beta)e^{\kappa_1+2\kappa_2}+2(1+\beta)e^{2\kappa_1+\kappa_2}+2(2+\beta)e^{\kappa_1}+2(3-\beta)e^{\kappa_2},\\
c_1&=-8e^{\kappa_1+\kappa_2},\\
a_2&=e^{2\kappa_1+2\kappa_2}+(1-2\beta)(e^{2\kappa_1}-e^{2\kappa_2})-1,\\
b_2&=-2\beta e^{\kappa_1+2\kappa_2}+2(\beta-1)e^{2\kappa_1+\kappa_2}+2\beta e^{\kappa_1}+2(1-\beta)e^{\kappa_2},\\
c_2&=0,
\end{aligned} \tag{3.8}$$

so that (3.6) reduces to

$$\hat{c}(q)=2\frac{a_1+b_1\cos q+c_1\cos^2 q}{a_2+b_2\cos q} \quad (3.9)$$

with a_1, b_1, c_1, a_2, and b_2 given by (3.8).

We remark that in (3.9) the numerator cannot be a multiple of the denominator because this would turn $\hat{c}(q)$ into the form $a'_1+b'_1\cos q$, and would imply

$$\hat{h}(q)=2\frac{a'_1+b'_1\cos q}{2-a'_1-b'_1\cos q} ,$$

which is incompatible with (3.5) when $\mathcal{J}_1$ and $\mathcal{J}_2$ are nonzero.

IV. ASYMPTOTIC DECAY

It is apparent from expression (3.9) for $\hat{c}(q)$ that the decay properties of the direct correlation function $c(|n|)$ for $|n|\to\infty$ will be determined by the nature of the root of the equation

$$a_2+b_2\cos q=0 , \quad (4.1)$$

where a_2 and b_2 are defined in (3.8). According to (3.8), a_2 and b_2 are functions of κ_1, κ_2, and β, and these are all, in turn, because of (2.2) and (2.3), functions of J_1, J_2, and T. We will find it more convenient to view a_2 and b_2 as functions of J_1, J_2, and T rather than as functions of κ_1, κ_2, and β.

If there are values of the couplings J_1 and J_2 and of the temperature T which are real and are such that the term $b_2=b_2(J_1,J_2,T)$ vanishes, then (3.9) will become

$$\hat{c}(q)=\frac{2}{a_2}(a_1+b_1\cos q+c_1\cos^2 q)$$

$$=\frac{2}{a_2}\left[a_1+\frac{c_1}{2}+b_1\cos q+\frac{c_1}{2}\cos 2q\right] . \quad (4.2)$$

Viewed as a function of the complex variable q, $\hat{c}(q)$ is then an entire function and comparison of (4.2) with (3.2) shows that $c(|n|)=0$ for $|n|>2$. Because $c(|n|)$ cannot vanish for $|n|<2$ when T is finite (see remark at the end of Sec. III), it then follows that $c(|n|)$ has exactly the range of the interactions.

If, on the other hand, there are no real values of the coupling constants J_1, J_2 and of the temperature T such that $b_2=b_2(J_1,J_2,T)$ vanishes, then $\hat{c}(q)$, viewed as a function of the complex variable q, has a pole given by the root of (4.1) and $c(|n|)$ will no longer vanish identically for $|n|>2$.

The remainder of this section is devoted to the discussion of these two cases $b_2=0$ and $b_2\neq 0$.

A. Case $b_2(J_1,J_2,T)=0$

In order to discuss the equation $b_2=0$ in terms of the couplings J_1 and J_2 and of the temperature T, we first rewrite b_2 as given in (3.8) by using the expressions for κ_1 and κ_2 as given in (2.2). The equation $b_2=0$ then becomes

$$-\beta\frac{\lambda^2}{\mu_+\mu_-^2}+(\beta-1)\frac{\lambda^2}{\mu_-\mu_+^2}+\beta\frac{1}{\mu_+}+(1-\beta)\frac{1}{\mu_-}=0 ,$$

which can be reexpressed as

$$\lambda^2[\beta\mu_+ +(1-\beta)\mu_-]=\mu_+\mu_-[\beta\mu_- +(1-\beta)\mu_+] . \quad (4.3)$$

Using the expressions for λ, $\mu_\pm$, and β given by (2.2) and (2.3), we find that (4.3) can be rewritten, after some algebra, as

$$x(x^2-1)^{1/2}[x^2(x^2-1)+y(1-y)]^{1/2}$$
$$-(x^2-y)^{1/2}][x+(x^2-1+y)^{1/2}]=0 , \quad (4.4)$$

where we have introduced

$$x\equiv\cosh\mathcal{J}_1 \quad (4.5)$$

and

$$y\equiv e^{-4\mathcal{J}_2} .$$

Observing that $x>0$, and discarding the solution $x=1$ which corresponds to $\mathcal{J}_1=0$, i.e., to $T=+\infty$, we see that Eq. (4.4) is equivalent to

$$[x^2(x^2-1)+y(1-y)]^{1/2}-(x^2-y)^{1/2}=0 ,$$

that is, to

$$x^2(x^2-2)=y(y-2) . \quad (4.6)$$

The only solution of (4.6) is

$$x^2=y , \quad (4.7)$$

since the equations $x^2=y-2$ and $x^2-2=y$ are incompatible.

With (4.5), result (4.7) reads

$$\cosh\mathcal{J}_1=e^{-2\mathcal{J}_2} ,$$

or, equivalently,

$$\cosh(J_1/k_BT)=e^{-2J_2/k_BT} . \quad (4.8)$$

For a given finite nonzero value of the temperature T, this equation will admit a solution J_1 in terms of J_2 (or vice versa), provided that J_1 and J_2 satisfy $0>J_2>-\frac{1}{2}|J_1|$. Alternatively, and perhaps more naturally, Eq. (4.8) can be viewed as an equation for T, given J_1 and J_2.

It remains to determine the behavior of the other terms a_1, b_1, b_2, and a_2 of $\hat{c}(q)$ [see (4.2)] when condition (4.8) is met.

We first note that when (4.8) holds, we have, according to (2.3),

$$\mu_+=\mu_-=\frac{\sinh\mathcal{J}_1}{(\cosh\mathcal{J}_1)^{1/2}}$$

and it follows, using (2.2), that

$$\kappa_1=\kappa_2\equiv\kappa=\ln\left[\cosh\mathcal{J}_1+\frac{[\cosh(2\mathcal{J}_1)]^{1/2}}{\sinh\mathcal{J}_1}\right] . \quad (4.9)$$

With (4.9), we then find from (3.8) that

$$a_1^*\equiv a_1(\kappa_1=\kappa_2=\kappa)=-e^{4\kappa}-4e^{2\kappa}-3 ,$$

$$b_1^*\equiv b_1(\kappa_1=\kappa_2=\kappa)=2e^{\kappa}(3e^{2\kappa}+5) , \quad (4.10)$$

$$c_1^*\equiv c_1(\kappa_1=\kappa_2=\kappa)=-8e^{2\kappa} ,$$

so that the numerator of $\hat{c}(q)$ is well behaved when (4.8) holds.

Concerning the term $a_2^* \equiv a_2(\kappa_1=\kappa_2=\kappa)$, we must evaluate [see (3.8)]

$$a_2^* = \lim_{\kappa_1\to\kappa_2} [e^{2\kappa_1+2\kappa_2}+(1-2\beta)(e^{2\kappa_1}-e^{2\kappa_2})-1]$$
$$=e^{4\kappa}-1+\lim_{\kappa_1\to\kappa_2}[(1-2\beta)(e^{2\kappa_1}-e^{2\kappa_2})] .$$

As $\kappa_1\to\kappa_2$, $\cosh\mathscr{J}_1-e^{-4\mathscr{J}_2}\to 0$, so that $\beta\to\infty$ [see (2.3)] and $e^{2\kappa_1}-e^{2\kappa_2}\to 0$, and, consequently, a_2^* appears indeterminate. But we have, using (2.2) and (2.3),

$$\beta\sim-\frac{1}{(\cosh^2\mathscr{J}_1-e^{-4\mathscr{J}_2})^{1/2}}$$

and

$$e^{2\kappa_1}-e^{2\kappa_2}\sim(\cosh^2\mathscr{J}_1-e^{-4\mathscr{J}_2})^{1/2} ,$$

so that a_2^* is actually a finite constant. A detailed calculation shows that

$$a_2^* = [\coth\mathscr{J}_1+(1+\coth^2\mathscr{J}_1)^{1/2}]^4-1$$
$$-4\frac{\coth^2\mathscr{J}_1}{(\cosh 2\mathscr{J}_1)^{1/2}}\{3\cosh^2\mathscr{J}_1-1$$
$$+2\cosh\mathscr{J}_1[\cosh(2\mathscr{J}_1)]^{1/2}\} . \tag{4.11}$$

We have therefore found that when the couplings J_1, J_2, and the temperature T are related to each other by Eq. (4.8), the Fourier transform $\hat{c}(q)$ assumes the form

$$\hat{c}(q)=\frac{2}{a_2^*}\left[a_1^*+\frac{c_1^*}{2}+b_1^*\cos q+\frac{c_1^*}{2}\cos(2q)\right] \tag{4.12}$$

with a_1^*, b_1^*, c_1^*, and a_2^* given by (4.10) and (4.11).

Equations (4.10) and (4.11) show that all coefficients appearing in (4.12) are nonzero so that, comparing (4.12) with (3.2), we have shown that if condition (4.8) holds, then

$$c(|n|)=0 \quad \text{for all } |n|>2$$

and

$$c(|n|)\neq 0 \quad \text{for } |n|=0,\ 1,\text{ and } 2 . \tag{4.13}$$

In other words, the range of c is *exactly* that of the interactions, neither longer nor shorter.

It may also be noted from (4.10) and (4.11) that

$$c(0)=\frac{2}{a_2^*}\left[a_1^*+\frac{c_1^*}{2}\right]$$

is always negative, whereas $c(1)$ is always positive. These properties of $c(|n|)$ may be compared to the results obtained by Percus[2(a)] for the Ising model with nearest-neighbor couplings only, where $c(0)$ is always negative, whereas $c(1)$ is always positive, just as they are here.

When condition (4.8) holds, i.e., when, for given J_1 and J_2 satisfying $0>J_2>-\frac{1}{2}|J_1|$, the temperature T crosses the value T^* defined by

$$\cosh^2(J_1/k_BT^*)=e^{4|J_2|/k_BT^*} ,$$

then the eigenvalues μ_+ and μ_-, given by (2.3) change from real to complex, or vice versa, depending on whether the temperature is increasing or decreasing. Correspondingly, the decay lengths κ_1^{-1} and κ_2^{-1} also change from real to complex, or vice versa, and the asymptotic behavior of the pair correlation function $h(|n|)$ changes from a monotonic exponential decay to an oscillatory exponential decay. This temperature T^* at which this change in the nature of the decay of the pair correlation function takes place was named a disorder point of the first kind by Stephenson.[11] However, it must be stressed that no singularities occur in the thermodynamic functions or in the correlation lengths at $T=T^*$.[11]

B. Case $b_2(J_1,J_2,T)\neq 0$

When $b_2\neq 0$, the function $\hat{c}(q)$, considered as a function of the complex variable q, is no longer analytic in the whole q plane. This is because when $b_2\neq 0$, the denominator of $\hat{c}(q)$, which is equal to $a_2+b_2\cos q$, vanishes when

$$q=q^*=\arccos\left[\frac{-a_2}{b_2}\right] . \tag{4.14}$$

Consequently, $\hat{c}(q)$ has a pole at $q=q^*$; this pole is simple provided that $|a_2/b_2|\neq 1$.

The nature of the asymptotic decay of the direct correlation function $c(|n|)$ is determined by the location of the pole q^* in the complex plane. It follows from the Paley-Wiener theorem that if q^* has a nonzero imaginary part, $c(|n|)$ will decay exponentially as $|n|\to\infty$. Three cases may occur.

In the first case, if q^* is pure imaginary, $c(|n|)$ will have a monotonic exponential decay, the decay length of which is equal to $1/|\mathrm{Im}q^*|$.

In the second case, if q^* has both a nonzero imaginary and a nonzero real part, $c(|n|)$ will also decay exponentially as $|n|\to\infty$, but the exponential tail will exhibit oscillations.

Finally, if q^* is pure real, i.e., if $\hat{c}(q)$ has a pole in the interval $(0,2\pi)$, $c(|n|)$ no longer decays exponentially and special care is required in calculating the Fourier inverse of $\hat{c}(q)$, which is defined by

$$c(|n|)=\int_0^{2\pi}dq\, e^{-iqn}\hat{c}(q)$$
$$=\int_0^{2\pi}dq\, e^{iqn}\hat{c}(q) , \tag{4.15}$$

where we have used the fact that $\hat{c}(q)=\hat{c}(-q)$.

Whether q^* is real or complex will depend on the strengths and signs of the coupling constants J_1,J_2 as well as on the value of the temperature T. When J_1, J_2, and T are such that

$$\cosh^2(J_1/k_BT)-e^{-4J_2/k_BT}>0 , \tag{4.16}$$

examination of (2.2) and (2.3) shows that κ_1 and β are real and that κ_2 is complex with e^{κ_2} real negative. It then follows from expressions (3.8) determining a_2 and b_2 that both a_2 and b_2 are real when condition (4.16) holds.

Alternatively, viewing inequality (4.16) as a condition for the couplings J_1 and J_2 to be fulfilled for all values of the temperature T, we may replace it by the simpler condition

$$J_2 > 0, \quad \text{for all } J_1 \ . \tag{4.17}$$

When condition (4.17) holds, the pole q^* given by (4.14) is either pure real or pure imaginary. This is because when (4.17) is satisfied, a_2 and b_2 are pure real, as we have just seen, and the identity

$$\mathrm{Im}\cos q^* = -\sin(\mathrm{Re}q^*)\sinh(\mathrm{Im}q^*) = 0 \tag{4.18}$$

implies that either $\mathrm{Re}q^* = 0$ or $\mathrm{Im}q^* = 0$.

We will now show that when condition (4.17) holds and when $T \neq 0$ (the case $T = 0$ will be treated in detail in Sec. V), then necessarily

$$|\cos q^*| = \left| \frac{a_2}{b_2} \right| > 1 \ . \tag{4.19}$$

The proof of this property is based on a *reductio ad absurdum.* Assume that inequality (4.19) is violated. Then the identity

$$\mathrm{Re}\cos q^* = -\cos(\mathrm{Re}q^*)\cosh(\mathrm{Im}q^*) \ , \tag{4.20}$$

together with identity (4.18), implies that $\mathrm{Re}\cos q^* = -\cos(\mathrm{Re}q^*)$, i.e., that q^* lies on the real axis in the interval $(0, 2\pi)$. Consider next (4.15) which reads, using (3.9)

$$c(|n|) = \int_0^{2\pi} \frac{a_1 + b_1\cos q + c_1\cos^2 q}{a_2 + b_2\cos q} e^{iqn} dq \ . \tag{4.21}$$

Since $|a_2/b_2| < 1$, the integrand has a pole at q^* located on the open interval of integration. Without any loss of generality we shall assume that $|a_2/b_2| \neq 1$, so that q^* is a simple pole. We note that there is also a second simple pole at $2\pi - q^*$. The integral (4.21) must be evaluated by taking its principal value according to Cauchy, which may be done by indenting the contour of integration and using the method of residues. We consider the following closed contour of integration Γ in the complex q plane which consists of the segment $\Gamma_1 = (0, 2\pi)$, the vertical segments Γ_2 and Γ_4 given by $\mathrm{Re}q = 0$ and $\mathrm{Re}q = 2\pi$, respectively, and the horizontal segment Γ_3 given by $\mathrm{Im}q = q_0 = \text{const}$. This contour is pictured in Fig. 1.

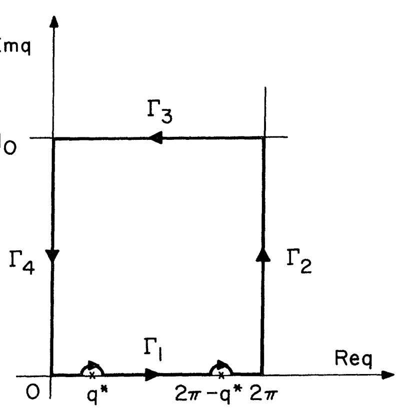

FIG. 1. Choice of contour of integration for evaluating the principal part of the integral (4.21).

The integrand in (4.21) is periodic of period 2π, so that the contributions on the two vertical segments, which are integrated upon in opposite directions, cancel each other. As we let q_0 tend to infinity, the contribution to the integral from Γ_3 becomes vanishingly small because of the factor

$$e^{iqn} = e^{i(\mathrm{Re}q + i\mathrm{Im}q)n} = e^{in\,\mathrm{Re}q} e^{-q_0 n} \ .$$

Since the integrand has no poles inside the closed contour Γ, we have[13]

$$c(|n|) = 2\pi i[\tfrac{1}{2}\mathrm{Res}(q^*) + \tfrac{1}{2}\mathrm{Res}(2\pi - q^*)] \ .$$

The residue at q^*, $\mathrm{Res}(q^*)$, is

$$2\frac{a_1 + b_1\cos q^* + c_1\cos^2 q^*}{b_2 \sin q^*} e^{iq^* n}$$

and since $\sin(2\pi - q^*) = -\sin q^*$, we find

$$c(|n|) = 2\pi i \left[\frac{a_1 + b_1\cos q^* + c_1\cos^2 q^*}{b_2\sin q^*} \right] \times (e^{iq^* n} - e^{-iq^* n})$$

$$= -4\pi \sin(q^* n) \frac{a_1 + b_1\cos q^* + c_1\cos^2 q^*}{b_2 \sin q^*} \ . \tag{4.22}$$

That the result (4.22) leads to a contradiction is most easily seen by considering the Ornstein-Zernike relation (3.1) which we rewrite as

$$c(|n|) = h(|n|) - \tfrac{1}{2} \sum_{n' \in Z} h(|n - n'|) c(|n'|) \ . \tag{4.23}$$

Clearly we have $h(|n|) < M < \infty$, so that

$$|c(|n|)| \leq |h(|n|)| + \frac{M}{2}\hat{c}(0) < \infty \ ,$$

because $\hat{c}(0) = 2\hat{h}(0)/[2 + \hat{h}(0)]$ is finite for all nonzero values of T. We can therefore take the limit $|n| \to \infty$ of both sides of (4.23), to get

$$\lim_{|n| \to \infty} \sum_{n' \in Z} h(|n - n'|) c(|n'|) = 0 \ ,$$

so that

$$\lim_{|n| \to \infty} c(|n|) = 0 \ ,$$

in contradiction to (4.22), as we wished to show. Consequently the pole q^* of $\hat{c}(q)$ cannot lie on the real axis, and must have a nonzero imaginary part. From (4.18) and (4.20) it then follows that q^* is pure imaginary and finally we conclude, by taking a closed contour around q^* and applying the residue theorem, that $c(|n|)$ has a monotonic exponential decay as $|n| \to \infty$.

Next we turn to the case where inequality (4.16) is reversed, i.e., where

$$\cosh^2(J_1/k_BT)-e^{-4J_2/k_BT}<0\ . \tag{4.24}$$

We shall again assume $T\neq0$, the case $T=0$ being dealt with in Sec. V. Note that for condition (4.24) to be satisfied for all values of T, we must have $0>J_2>-\frac{1}{2}|J_1|$.

When condition (4.24) holds, examination of Eqs. (2.2) and (2.3) reveals that κ_1 and κ_2 are no longer pure real but are now complex conjugate. We write accordingly

$$e^{\kappa_1}=\frac{\lambda}{\mu}e^{i\varphi}\ ,\qquad e^{\kappa_2}=\frac{\lambda}{\mu}e^{-i\varphi} \tag{4.25}$$

with μ the modulus of $\mu_\pm$ in (2.3).

To determine the nature of the asymptotic decay of $c(|n|)$, we need to know the complex character of the ratio $-a_2/b_2$ with a_2 and b_2 complex. We first determine the imaginary part of $-a_2/b_2$. Using (4.25), we have

$$\frac{a_2}{b_2}=\frac{1}{2}\frac{\frac{\lambda^4}{\mu^4}+\frac{\lambda^2}{\mu^2}(e^{2i\varphi}-e^{-2i\varphi})(1-2\beta)-1}{\beta\frac{\lambda^3}{\mu^3}(e^{i\varphi}-e^{-i\varphi})+\beta\frac{\lambda}{\mu}(e^{i\varphi}-e^{-i\varphi})-\frac{\lambda^3}{\mu^3}e^{i\varphi}+\frac{\lambda}{\mu}e^{-i\varphi}}\ .$$

Multiplying numerator and denominator by the complex conjugate of the latter and observing that $\mathrm{Re}\beta=\frac{1}{2}$, we find that

$$\mathrm{Im}(a_2/b_2)=0$$

if and only if

$$\left[1+\frac{\lambda^2}{\mu^2}\right]\left[\frac{\lambda}{\mu}-2\,\mathrm{Re}\beta\right]\left[\frac{\lambda^4}{\mu^4}-4\frac{\lambda^2}{\mu^2}(\mathrm{Im}\beta)\sin(2\varphi)-1\right]=0\ . \tag{4.26}$$

Clearly the first factor is nonzero and since $2\,\mathrm{Re}\beta=1$ and $\lambda/\mu>1$ (when $T\neq0$) [see (2.3)], so is the second. Noting that

$$\sin(2\varphi)=\frac{\mathrm{Im}(\mu_+^2)}{\mu^2}=2\frac{\mathrm{Im}\mu_+\,\mathrm{Re}\mu_+}{\mu^2}$$

and using

$$\mathrm{Im}\beta=\frac{1}{4}\frac{\sinh(2\mathcal{J}_1)}{(\sinh^2\mathcal{J}_1+e^{-4\mathcal{J}_2})^{1/2}(-\cosh^2\mathcal{J}_1+e^{-4\mathcal{J}_2})^{1/2}}\ , \tag{4.27}$$

which follows from (2.2) and (2.3), we find, after some algebra, that

$$\mathrm{Im}(a_2/b_2)=0$$

if and only if

$$e^{-4\mathcal{J}_2}=0\ ,$$

i.e., $\mathcal{J}_2=+\infty$. But this contradicts the assumption that $\cosh^2\mathcal{J}_1-e^{-4\mathcal{J}_2}<0$, and we conclude that $\mathrm{Im}(a_2/b_2)$ can never vanish whenever condition (4.24) holds and T is nonzero.

Finally, we discuss the equation $\mathrm{Re}(a_2/b_2)=0$. From the previous discussion of the equation $\mathrm{Im}(a_2/b_2)=0$, it may be shown that

$$\mathrm{Re}(a_2/b_2)=0$$

if and only if

$$-2\,\mathrm{Im}\beta\sin\varphi\left[1+\frac{\lambda^2}{\mu^2}\right]-\frac{\lambda}{\mu}\left[\frac{\lambda^2}{\mu^2}-1\right]\cos\varphi=0\ . \tag{4.28}$$

Since, on the one hand, $\mathrm{Im}\beta>0$ [see (4.27)] and on the other hand $0<\varphi<(\pi/2)$ and $(\lambda^2/\mu^2)-1>0$ when $T\neq0$, both terms of the left-hand side of (4.28) are always negative and consequently (4.28) can never be satisfied. We therefore conclude that $\mathrm{Re}(a_2/b_2)$ can never vanish. Together with the previous result that $\mathrm{Im}(a_2/b_2)$ never vanishes either, this establishes that when condition (4.24) holds, $c(|n|)$ has an exponential decay which is always oscillatory.

We conclude this section by discussing the limiting behavior of $c(|n|)$ as $T\to+\infty$. As $T\to+\infty$, examination of (2.2) and (2.3) shows that both κ_1 and κ_2 diverge, so that both ξ_1 and ξ_2 vanish, in accord with intuition. Consequently, we have from (2.1) that as $T\to+\infty$, $h(|n|)\to0$ for all $|n|\neq0$. The behavior of $c(|n|)$ is found from the Ornstein-Zernike relation (3.1) in which we set $|n|\neq0$ and define $n''\equiv n-n'$, to get

$$\begin{aligned}0&=c(|n|)+\tfrac{1}{2}\sum_{n''\in Z}h(|n''|)c(|n-n''|)\\&=c(|n|)+\tfrac{1}{2}h(0)c(|n|)\\&=\tfrac{1}{2}c(|n|)\ ,\end{aligned}$$

where we have made use of the identity $h(0)\equiv-1$ (see Sec. III).

The behavior of $c(|n|)$ at the origin is obtained by setting $n=0$ in (3.1) and making use again of $h(0)\equiv-1$. We have

$$\begin{aligned}-1&=c(0)+\tfrac{1}{2}\sum_{n'\in Z}h(|n'|)c(|n'|)\\&=c(0)-\tfrac{1}{2}c(0)\ ,\end{aligned}$$

so that

$$c(0)=-2\ .$$

Therefore as $T\to+\infty$, we get

$$c(|n|)=0,\ \text{all}\ |n|\neq0\ ,$$

and (4.29)

$$c(0)=-2\ .$$

The range of the direct correlation function therefore reduces to naught as the temperature increases without limit, in accord with one's expectation. When only nearest-neighbor interactions are present, precisely the same exact result (4.29) holds.[2(a)]

It may be noted that (4.29) is consistent with the earlier result (4.13) derived in Sec. IV A; this is because condition (4.8) is trivially satisfied in the limit as $T\to+\infty$.

V. CRITICAL BEHAVIOR

Because the linear model we are considering has finite-range forces, a phase transition from a disordered to an ordered state can only occur at $T=0$.

In the present model, which, for convenience, will now be discussed in magnetic language, $T=0$ is a critical point for all values of J_1 and J_2 except when $J_2=-\frac{1}{2}|J_1|$, the ground state being ferromagnetic in all cases except when $J_2<-\frac{1}{2}|J_1|$, where the next-nearest-neighbor coupling is strong enough to make the ground state antiferromagnetic.[11]

As the critical point $T_c=0$ is approached, the correlation length increases and at $T=0$ it ultimately diverges, the pair correlation function $h(|n|)$ assuming the simple form $h(|n|)=1$ for all $|n|>0$ when the ground state is ferromagnetic, and $h(|n|)=(-1)^{|n|/2}$ for even n and $h(|n|)=0$ for odd n when the ground state is antiferromagnetic. But what happens to the direct correlation function is far from being so obvious.

We shall determine the behavior of $c(|n|)$ as $T\to0^+$ by examining the limiting behavior, as $T\to0^+$, of each term of $c(|n|)$ as given by (3.8) and (3.9), and distinguishing in Secs. V A and V B the cases where the ground state is, respectively, ferromagnetic and antiferromagnetic. Finally, we discuss in Sec. V C the critical behavior of the second moment of $c(|n|)$.

A. Ferromagnetic ground state

We first examine the behavior of the denominator of $\hat{c}(q)$ as given by (3.9). When $J_1,J_2>0$, all quantities, except κ_2, are real; κ_2 is complex because μ_- is negative for $J_2>0$ [see (2.2) and (2.3)].

As $T\to0$, $e^{-4\mathcal{J}_2}$ vanishes while $\cosh\mathcal{J}_1$ and $\sinh\mathcal{J}_1$ diverge. This suggests expanding all quantities in the parameter $e^{-4\mathcal{J}_2}\ll1$. We find, to first order in $e^{-4\mathcal{J}_2}$,

$$\beta=4e^{-4\mathcal{J}_1-4\mathcal{J}_2}\ ,$$

$$e^{\kappa_1}=1+2e^{-2\mathcal{J}_1-4\mathcal{J}_2}\ ,$$

$$e^{\kappa_2}=-e^{-2\mathcal{J}_1}\ ,$$

from which we calculate a_2 and b_2 as given by (3.8). We obtain

$$a_2=4e^{-8\mathcal{J}_2}+4e^{2\mathcal{J}_1-4\mathcal{J}_2}+4e^{-4\mathcal{J}_1-8\mathcal{J}_2}-8e^{-4\mathcal{J}_1-4\mathcal{J}_2}-32e^{-8\mathcal{J}_1-12\mathcal{J}_2}-32^{-6\mathcal{J}_1-8\mathcal{J}_2}+8e^{-4\mathcal{J}_2} \quad (5.1)$$

and

$$b_2=-8e^{-2\mathcal{J}_1-8\mathcal{J}_2}+16e^{-6\mathcal{J}_1-8\mathcal{J}_2}-32e^{-6\mathcal{J}_1-12\mathcal{J}_2}-32e^{-4\mathcal{J}_1-8\mathcal{J}_2}+8e^{-4\mathcal{J}_1-4\mathcal{J}_2}\ ,$$

from which it follows that

$$\lim_{T\to0^+}\frac{a_2}{b_2}=\lim_{T\to0^+}\left(-\tfrac{1}{2}e^{4\mathcal{J}_1+4\mathcal{J}_2}\right)=-\infty\ . \quad (5.2)$$

Next we turn to the numerator of $\hat{c}(q)$ and expand all terms in powers of $e^{-4\mathcal{J}_2}$. We find

$$\begin{aligned}a_1=&-4e^{4\mathcal{J}_1}-4e^{2\mathcal{J}_1-4\mathcal{J}_2}+8e^{-4\mathcal{J}_2}-4e^{-8\mathcal{J}_2}-4e^{-2\mathcal{J}_1-4\mathcal{J}_2}-8e^{-4\mathcal{J}_1-4\mathcal{J}_2}-4e^{-4\mathcal{J}_1-8\mathcal{J}_2}\\&-32e^{-6\mathcal{J}_1-8\mathcal{J}_2}-32e^{-8\mathcal{J}_1-12\mathcal{J}_2}-4\ ,\\b_1=&4e^{4\mathcal{J}_1}-8e^{2\mathcal{J}_1}+8e^{2\mathcal{J}_1-4\mathcal{J}_2}-24e^{-2\mathcal{J}_1-8\mathcal{J}_2}+8e^{-4\mathcal{J}_1-4\mathcal{J}_2}\\&-32e^{-4\mathcal{J}_1-8\mathcal{J}_2}-32e^{-6\mathcal{J}_1-12\mathcal{J}_2}+16e^{-6\mathcal{J}_1-8\mathcal{J}_2}+8e^{-2\mathcal{J}_1-4\mathcal{J}_2}-16e^{-4\mathcal{J}_2}+4\ ,\end{aligned} \quad (5.3)$$

and

$$c_1=8e^{2\mathcal{J}_1}+16e^{-4\mathcal{J}_2}\ .$$

Combining (5.3) and (5.2) gives, to leading order,

$$\frac{a_1}{a_2}=-e^{2\mathcal{J}_1+4\mathcal{J}_2}-1\ ,$$

$$\frac{b_1}{a_2}=e^{2\mathcal{J}_1+4\mathcal{J}_2}-2e^{4\mathcal{J}_2}+2\ , \quad (5.4)$$

and

$$\frac{c_1}{a_2}=2e^{4\mathcal{J}_2}\ .$$

Finally, inserting results (5.1)–(5.4) into expression (3.9) for $\hat{c}(q)$ gives the desired answer:

$$\hat{c}(q)\underset{T\to0^+}{\cong}-2(e^{2\mathcal{J}_1+4\mathcal{J}_2}-e^{4\mathcal{J}_2}+1)+2(e^{2\mathcal{J}_1+4\mathcal{J}_2}-2e^{4\mathcal{J}_2}+2)\cos q+2e^{4\mathcal{J}_2}\cos 2q\ . \quad (5.5)$$

Comparison of (5.5) with (3.2) shows that the direct correlation function $c(|n|)$ is given by

$$c(|n|) \underset{T\to 0^+}{\cong} \begin{cases} -2(e^{2\mathcal{J}_1+4\mathcal{J}_2}-e^{4\mathcal{J}_2}+1) & \text{for } |n|=0 \\ e^{2\mathcal{J}_1+4\mathcal{J}_2}+2-2e^{4\mathcal{J}_2} & \text{for } |n|=1 \\ e^{4\mathcal{J}_2} & \text{for } |n|=2 \\ 0 & \text{for all } |n|>2. \end{cases} \tag{5.6}$$

As $T\to 0^+$, $c(0)$, $c(1)$, and $c(2)$ are all seen to diverge; but while

$$\lim_{T\to 0^+} \frac{c(0)}{c(1)} = -2 , \tag{5.7}$$

$$\lim_{T\to 0^+} \frac{c(1)}{c(2)} = +\infty , \tag{5.8}$$

so that as $T\to 0^+$, $c(0)$ and $c(1)$ are both of the same strength, while $c(2)$ becomes negligible compared to either of them.

It may also be noted that in the present case where $\mathcal{J}_1,\mathcal{J}_2>0$, $h(|n|)\equiv 1$ at $T=0$, and therefore

$$\hat{h}(q=0)=\sum_{n\in Z} h(|n|)=+\infty ,$$

so that it follows from (3.3) that

$$\hat{c}(q=0)=2,\quad T=0 . \tag{5.9}$$

As explained earlier in Sec. III, (5.9) is the special case $\rho=\frac{1}{2}$ of the more general relation[1]

$$\hat{c}(q=0)=\rho^{-1} ,$$

which holds at the critical point of a fluid of density ρ.

Relation (5.9) provides a useful consistency check of the expressions (5.1)–(5.3) we derived above. From (3.6) we have

$$\hat{c}(q=0)=2\frac{a_1+b_1+c_1}{a_2+b_2} , \tag{5.10}$$

and from (5.1)–(5.3) we find that as $T\to 0^+$,

$$a_1+b_1+c_1 \sim 4e^{2\mathcal{J}_1-4\mathcal{J}_2}$$

and

$$a_2+b_2 \sim 4e^{2\mathcal{J}_1-4\mathcal{J}_2} ,$$

so that (5.10) becomes, at $T=0$,

$$\hat{c}(q=0)=2 ,$$

in agreement with (5.9).

Alternatively, we can use result (5.6) in conjunction with the relation

$$\hat{c}(q=0)=c(0)+2c(1)+2c(2) ,$$

which follows directly from definition (3.2), to get

$$\begin{aligned}\hat{c}(q=0) &= -2e^{2\mathcal{J}_1+4\mathcal{J}_2}-2+2e^{4\mathcal{J}_2} \\ &\quad +2e^{2\mathcal{J}_1+4\mathcal{J}_2}-4e^{4\mathcal{J}_2}+4 \;+2e^{4\mathcal{J}_2} \\ &=2 ,\end{aligned}$$

again reproducing (5.9), as it should.

Finally, it will be observed that the case $\mathcal{J}_1>0,\mathcal{J}_2<0$, with $|\mathcal{J}_2|<\mathcal{J}_1/2$, which also yields a ferromagnetic ground state at $T=0$, reduces to the case $J_1,J_2>0$, which we have just dealt with. The reason for this is that expressions of the form $e^{-4\mathcal{J}_2}/\sinh^2\mathcal{J}_1$ or $e^{-4\mathcal{J}_2}/\cosh^2\mathcal{J}_1$, in terms of which $\hat{c}(q)$ was expanded, behave, as $T\to 0^+$, as $\frac{1}{2}e^{-4\mathcal{J}_2-2\mathcal{J}_1}$ and therefore vanish as $T\to 0^+$ provided that $-4\mathcal{J}_2-2\mathcal{J}_1<0$, i.e., that $-\mathcal{J}_2=|\mathcal{J}_2|<(\mathcal{J}_1/2)$. And this last condition is precisely that which guarantees the ferromagnetic character of the ground state.

B. Antiferromagnetic ground state

When $|\mathcal{J}_2|>\mathcal{J}_1/2$, examination of (2.2) and (2.3) shows that the appropriate small parameter in terms of which $\hat{c}(q)$ is to be expanded near $T=0$ is of the form $\sinh^2\mathcal{J}_1/e^{-4\mathcal{J}_2}$ or $\cosh^2\mathcal{J}_1/e^{-4\mathcal{J}_2}$: Both of these behave as $\frac{1}{4}e^{2\mathcal{J}_1-4|\mathcal{J}_2|}$ when $T\to 0^+$, and $e^{2\mathcal{J}_1-4|\mathcal{J}_2|}$ vanishes, as $T\to 0^+$, whenever $2\mathcal{J}_1-4|\mathcal{J}_2|<0$, i.e., precisely when $|\mathcal{J}_2|>\mathcal{J}_1/2$.

In order to determine the behavior of $\hat{c}(q)$ as $T\to 0^+$, we shall first need (see Sec. IV) the expansions of λ/μ, $\mathrm{Im}\beta$, $e^{\pm i\varphi}$, and $e^{\pm 2i\varphi}$ in terms of the small parameter $(e^{\mathcal{J}_1-2|\mathcal{J}_2|})^2$, the notations being those introduced in (4.25).

We find

$$\begin{aligned}\frac{\lambda}{\mu} &= 1+\tfrac{1}{2}e^{\mathcal{J}_1-2|\mathcal{J}_2|}+\tfrac{1}{8}e^{2\mathcal{J}_1-4|\mathcal{J}_2|} , \\ \mathrm{Im}\beta &= \tfrac{1}{8}e^{2\mathcal{J}_1-4|\mathcal{J}_2|}-\frac{1}{8^3}e^{6\mathcal{J}_1-12|\mathcal{J}_2|} , \\ e^{\pm i\varphi} &= (\tfrac{1}{2}e^{\mathcal{J}_1-2|\mathcal{J}_2|}+\tfrac{1}{4}e^{\mathcal{J}_1-6|\mathcal{J}_2|}) \\ &\quad \mp i(1-\tfrac{1}{8}e^{2\mathcal{J}_1-4|\mathcal{J}_2|}+\tfrac{1}{2}e^{-4|\mathcal{J}_2|}-\tfrac{1}{16}e^{2\mathcal{J}_1-8|\mathcal{J}_2|}) ,\end{aligned} \tag{5.11}$$

and

$$\begin{aligned}e^{\pm i2\varphi} &= -(1-\tfrac{1}{2}e^{2\mathcal{J}_1-4|\mathcal{J}_2|}+e^{-4|\mathcal{J}_2|}-\tfrac{1}{2}e^{2\mathcal{J}_1-8|\mathcal{J}_2|}) \\ &\quad \mp i(e^{\mathcal{J}_1-2|\mathcal{J}_2|}-\tfrac{1}{8}e^{3\mathcal{J}_1-6|\mathcal{J}_2|} \\ &\quad +e^{\mathcal{J}_1-6|\mathcal{J}_2|}-\tfrac{1}{8}e^{3\mathcal{J}_1-10|\mathcal{J}_2|}) .\end{aligned}$$

Let us first discuss the denominator of $\hat{c}(q)$. Using (4.25) and (3.8), we may rewrite a_2 and b_2 as

$$a_2=\left[\frac{\lambda}{\mu}\right]^4+2i(1-2\beta)\left[\frac{\lambda}{\mu}\right]^2\sin(2\varphi)-1 ,$$

and

$$\begin{aligned}\tfrac{1}{2}b_2 &= 2i\beta\left[\frac{\lambda}{\mu}\right]^3\sin\varphi+2i\beta\frac{\lambda}{\mu}\sin\varphi \\ &\quad -\left[\frac{\lambda}{\mu}\right]^3 e^{i\varphi}+\frac{\lambda}{\mu}e^{-i\varphi} .\end{aligned}$$

For a_2 we then obtain, using (5.11),

$$a_2=2e^{\mathcal{J}_1-2|\mathcal{J}_2|} , \tag{5.12}$$

while the first term of $\frac{1}{2}b_2$ becomes

$$\tfrac{1}{4}e^{2\mathscr{J}_1-4|\mathscr{J}_2|}-i(1+\tfrac{3}{2}e^{\mathscr{J}_1-2|\mathscr{J}_2|}) ,$$

the second

$$-\tfrac{1}{2}e^{\mathscr{J}_1-2|\mathscr{J}_2|}+i(1+\tfrac{3}{2}e^{\mathscr{J}_1-2|\mathscr{J}_2|}) ,$$

the third

$$\tfrac{1}{4}e^{2\mathscr{J}_1-4|\mathscr{J}_2|}-i(1+\tfrac{1}{2}e^{\mathscr{J}_1-2|\mathscr{J}_2|})$$

and the fourth

$$\tfrac{1}{2}e^{\mathscr{J}_1-2|\mathscr{J}_2|}+i(1+\tfrac{1}{2}e^{\mathscr{J}_1-2|\mathscr{J}_2|}) ,$$

so that

$$b_2=e^{2\mathscr{J}_1-4|\mathscr{J}_2|} . \tag{5.13}$$

Combining (5.12) and (5.13) we get

$$\lim_{T\to 0^+}\frac{a_2}{b_2}=\lim_{T\to 0^+}2e^{-\mathscr{J}_1+2|\mathscr{J}_2|}=+\infty . \tag{5.14}$$

Consequently, as $T\to 0^+$, the pole of $\hat{c}(q)$ moves arbitrarily far from the real axis, signaling, just as in the ferromagnetic case dealt with in Sec. V A [see (5.2)], a strictly finite range of $c(|n|)$ in direct space.

The detailed behavior of $c(|n|)$ is determined by analyzing the terms a_1, b_1, and c_1. It is found that, as $T\to 0^+$,

$$a_1=2e^{\mathscr{J}_1-2|\mathscr{J}_2|}(1-e^{\mathscr{J}_1-2|\mathscr{J}_2|}-e^{2\mathscr{J}_1-4|\mathscr{J}_2|}) ,$$

$$b_1=4e^{\mathscr{J}_1-2|\mathscr{J}_2|}(2+e^{\mathscr{J}_1-2|\mathscr{J}_2|}) , \tag{5.15}$$

and

$$c_1=-8(1+e^{\mathscr{J}_1-2|\mathscr{J}_2|}) .$$

Because

$$\lim_{T\to 0^+}\frac{b_2}{a_2}=0$$

[see (5.14)], expression (3.9) for $\hat{c}(q)$ reduces to (4.2) and results (5.12), (5.13), and (5.15), when combined with definition (3.2), imply that

$$c(|n|)\underset{T\to 0^+}{\cong}\begin{cases}-4e^{2|\mathscr{J}_2|-\mathscr{J}_1} & \text{for } |n|=0\\ +4+2e^{\mathscr{J}_1-2|\mathscr{J}_2|} & \text{for } |n|=1\\ -2e^{2|\mathscr{J}_2|-\mathscr{J}_1} & \text{for } |n|=2\\ 0 \text{ for } |n|>2. \end{cases} \tag{5.16}$$

As $T\to 0^+$, $c(1)$ tends to the constant $+4$, while $c(0)$ and $c(2)$ both diverge negatively at the same rate:

$$\lim_{T\to 0^+}\frac{c(0)}{c(2)}=2 . \tag{5.17}$$

Result (5.17) may be compared to (5.7), its analog for the case of a ferromagnetic ground state. Results (5.7) and (5.17) may be understood intuitively as follows. As $T\to 0^+$, the nature of the ground state is determined by the strongest of the two coupling constants J_1 and J_2: When the ground state is ferromagnetic, the correlation is governed by J_1, while it is governed by J_2 when the ground state is antiferromagnetic. Indeed, in the latter case, there is no correlation between nearest-neighbor particles (spins) at $T=0$, so that results (5.17) and (5.7) may be considered to be similar, the opposite signs reflecting the opposite nature of the correlation between pairs of nearest-correlated particles (spins) at $T=0$.

It will finally be noted that although in the present case $T=0$ is a critical point, the relation $\hat{c}(q=0)=\frac{1}{2}$ does not hold, in contrast to the situation prevailing in the previous case [cf. (5.9)]. Indeed, we find here that

$$\lim_{T\to 0^+}\hat{c}(q=0)=2\lim_{T\to 0^+}\left[\frac{a_1+b_1+c_1}{a_2}\right]$$
$$=2\lim_{T\to 0^+}(-8e^{2|\mathscr{J}_2|-\mathscr{J}_1})$$
$$=-\infty .$$

The reason for this result is simply that at $T=0$, we no longer have $\hat{h}(q=0)=+\infty$, as we did when $\mathscr{J}_1>2|\mathscr{J}_2|$, but rather

$$\hat{h}(q=0)=\sum_{n\in Z}h(|n|)$$
$$=-1+2\sum_{\substack{n\in Z\setminus\{0\}\\ n\text{ even}}}(-1)^{|n|/2} ,$$

which oscillates finitely.[14]

C. Second moment of the direct correlation function

The second moment A of the direct correlation function is defined by

$$A=\tfrac{1}{2}\sum_{n\in Z}c(|n|)|n|^2 , \tag{5.18}$$

which is the discrete, one-dimensional version of the expression of the second moment of the direct correlation function,

$$A=\frac{1}{2d}\int c(|r|)|r|^2 d^d r ,$$

appropriate to a spatially uniform d-dimensional fluid.

To determine the critical behavior of A, direct use will be made of the fact, established in Secs. V A and V B, that as the critical point is approached, the direct correlation function acquires exactly the range of the interactions. Consequently, Eq. (5.18) becomes, as $T\to 0^+$,

$$A=\tfrac{1}{2}[0c(0)+2c(1)+8c(2)]$$
$$=c(1)+4c(2) , \tag{5.19}$$

with $c(1)$ and $c(2)$ given by (5.6) or (5.16), depending on whether the phase transition occurring at $T=0$ is of the ferromagnetic or antiferromagnetic type.

When the ground state is ferromagnetic, we find, inserting (5.6) into (5.19),

$$A_{\text{ferro}}=e^{2\mathscr{J}_1+4\mathscr{J}_2} \text{ as } T\to 0^+ , \tag{5.20}$$

while when the ground state is antiferromagnetic, we get, combining (5.16) and (5.19),

$$A_{\text{antiferro}} = -8e^{2|\mathcal{J}_2|-\mathcal{J}_1} \text{ as } T\to 0^+ . \tag{5.21}$$

Finally, we shall use results (5.20) and (5.21) to test the scaling prediction that as the critical point of a d-dimensional system is approached, one should have[15]

$$A = c\xi^{+\eta} \tag{5.22}$$

with ξ the correlation length of the spontaneous density (spin) fluctuations in the system, η the critical exponent measuring the departure from mean-field behavior of the asymptotic decay of the pair correlation function at the critical point, and c a nonuniversal constant which depends on the details of the system.

The behavior of the correlation length ξ as the critical point is approached is readily extracted from the above results. We shall denote the correlation length ξ by ξ_{ferro} ($\xi_{\text{antiferro}}$) when the system undergoes a ferromagnetic (antiferromagnetic) phase transition at $T=0$.

As we saw at the beginning of this section, the divergence of ξ_{ferro} at $T=0$ is induced by the eigenvalue ratio λ/μ_+ approaching unity as $T\to 0^+$. From definition (2.2) we get

$$\xi_{\text{ferro}} = \left[\ln\frac{\lambda}{\mu_+}\right]^{-1}_{\text{ferro}}$$

and from the result $(e^{\kappa_1})_{\text{ferro}} \sim 1+2e^{-2\mathcal{J}_1-4\mathcal{J}_2}$, which was derived earlier in Sec. V A, we find

$$\xi_{\text{ferro}} = \tfrac{1}{2}e^{2\mathcal{J}_1+4\mathcal{J}_2} \to +\infty \text{ as } T\to 0^+ . \tag{5.23}$$

As regards $\xi_{\text{antiferro}}$, it follows from definition (2.2) and results (4.25) and (5.11) that as $T\to 0^+$,

$$\begin{aligned}\xi_{\text{antiferro}} &= [\ln(1+\tfrac{1}{2}e^{\mathcal{J}_1-2|\mathcal{J}_2|})]^{-1} \\ &\sim 2e^{2|\mathcal{J}_2|-\mathcal{J}_1} \to +\infty .\end{aligned} \tag{5.24}$$

Combining (5.20) with (5.23) and (5.21) with (5.24), respectively, we get the desired relations:

$$A_{\text{ferro}} = \tfrac{1}{2}\xi_{\text{ferro}} \tag{5.25}$$

and

$$A_{\text{antiferro}} = -4\xi_{\text{antiferro}} . \tag{5.26}$$

We thus confirm the scaling prediction (5.22) with $\eta=1$. And we note that $\eta=1$ is the exact value of the critical exponent η in one-dimensional systems with short-range forces as follows trivially from the mere definition of η and the fact that at $T=0$, $h_{\text{ferro}}(|n|)\equiv 1$ for all n and $h_{\text{antiferro}}(|n|)=0$ for $|n|$ odd and $h_{\text{antiferro}}(|n|)=(-1)^{|n|/2}$ for $|n|$ even.

It may be mentioned that the scaling prediction (5.22) has also recently been confirmed, in another context, for the simpler model of a lattice gas with interactions restricted to nearest neighbors.[16] For that model it was found that (5.22) holds with the nonuniversal constant c equal to 2.

VI. SUMMARY AND DISCUSSION

We have presented an exact calculation of the direct correlation function of the one-dimensional lattice-gas (Ising) model with both nearest-neighbor and next-nearest-neighbor interactions, with special emphasis on its asymptotic decay and its behavior near and at the critical point, which occurs at zero temperature.

Depending on the value of the temperature and on the strengths and signs of the coupling constants, it has been found that the direct correlation function can either vanish exponentially at infinity, with an asymptotic decay which is either monotonic or oscillatory, or can have a strictly finite range which is exactly equal to that of the interactions. Moreover, we have seen that whenever the asymptotic decay of the direct correlation function is monotonic or oscillatory, so is that of the pair correlation function.[17]

A remarkable exception to this similarity between the asymptotic decay of the direct and the pair correlation functions occurs when the nearest-neighbor and next-nearest-neighbor couplings, denoted J_1 and J_2, respectively, satisfy the condition $0>J_2>-\frac{1}{2}|J_1|$. In that case, there is a unique value T^* of the temperature T at which the direct correlation function no longer decays exponentially at infinity, but has a strictly finite range exactly equal to that of the interactions. For all $T<T^*$, the direct correlation function has a monotonic exponential decay while for all $T>T^*$, its exponential decay is oscillatory. The same qualitative change in the nature of the asymptotic decay characterizes the pair correlation function with the fundamental difference that when $T=T^*$, it still decays exponentially,[11] unlike the direct correlation function. The transition in the character of the asymptotic decay which takes place at T^* is therefore more pronounced for the direct correlation function than for the pair correlation function.

At the critical point, which occurs at $T=0$, the direct correlation function always has a finite range which is identical to that of the interactions. This exact result is in full agreement with one of the central ideas of the Ornstein-Zernike theory of critical fluctuations, in which it is assumed that the direct correlation function remains of finite range at the critical point.

However, while the range of the direct correlation function reduces to that of the interactions as the critical point is approached, at the same time the values assumed by the direct correlation function become unbounded.

That is to say, at the critical point, particles (spins) which do not interact directly through the interaction couplings are also no longer "directly" correlated, while those particles (spins) which do interact directly become infinitely strongly "directly" correlated. In contrast to its strictly finite range at the critical point, the unboundedness of the direct correlation function at the critical point does contradict another central assumption of the Ornstein-Zernike theory according to which, at the critical point, the direct correlation function admits a Fourier transform which is analytic, and therefore bounded, at the origin.

The second moment of the direct correlation function has been shown to become increasingly large as the critical point is approached, ultimately diverging at the critical point itself. Moreover, the second moment of the direct correlation function has been found to diverge proportionally to the correlation length of the spontaneous density (spin) fluctuations, confirming a prediction of scaling theory in one dimension.

That the second moment of the direct correlation function of a system exhibiting nonclassical critical behavior diverges at the critical point had been proposed by Green.[18(a)] But in the present model this divergence does not occur by Green's mechanism, according to which the divergence of the second moment of the direct correlation function is due to the slow asymptotic decay of that function, predicted[18(b)] to be inversely proportional to the distance squared in one dimension. As the present exact results demonstrate, the divergence of the second moment of the direct correlation function is not induced by the change of the asymptotic decay of that function from an exponential to a power-law-like form, but rather by the values of the direct correlation function itself which become unbounded at the critical point, while at the same time the range of the direct correlation function becomes equal to that of the interactions. It should be observed that such lack of boundedness of the direct correlation function is not *a priori* prevented by the definition of this function: The direct correlation function lacks the obvious physical interpretation of the usual pair correlation function and is, in particular, not restricted to remain finite, since it is not, unlike the pair correlation function, defined as a probability.

Clearly, the exact results obtained here cannot adequately describe all the details of the behavior of more realistic systems. First, in real systems, the oscillations in the tail of the pair correlation function are induced by the hard core of the molecules. But in the present model, the oscillations in the tails of the pair and direct correlation functions are not produced by the hard core, which is here trivially imposed by the lattice rather than by the particles themselves,[19] but by the differing signs of the coupling constants. Evidently, in lattice systems an extended core is necessary to imitate the hard core of a real particle.[20] Second, it should also be recalled that the interactions in real systems often decay like power laws at infinity, so that the monotonic or oscillatory exponential asymptotic decay discussed above will not be seen in these systems in the truly asymptotic regime.[21]

It appears reasonable to assume that the results found here should remain valid in more general linear lattice systems with finite-range interactions and, on the basis of universality, one may also conjecture that the critical behavior found here may also be that of linear continuous systems with finite-range interactions. It would also be interesting, following the studies of Percus,[5–7] to see whether or not the results found here are affected by the presence of an external field.

Further rigorous work on models exhibiting nonclassical values of the critical exponents will be required to know whether the properties of the direct correlation function described above are restricted to one-dimensional systems or whether they do have a more general validity.

It may be mentioned that for Ornstein-Zernike systems, in which the direct correlation function $c(n)$ is related to the intermolecular potential $\Phi(n)$ by

$$c(n) \sim -\frac{1}{k_B T}\Phi(n)$$

for all values of the temperature, Stell has shown[8,22] that for one or two dimensions of space and for $\Phi(n)$ restricted to nearest-neighbor molecules, c necessarily becomes unbounded at the critical point which must then occur at zero absolute temperature.

ACKNOWLEDGMENTS

The author is indebted to B. Widom for a critical reading of the manuscript and for several clarifying questions. He is very grateful to J. K. Percus for stimulating and illuminating conversations, to T. Charbel for a useful discussion, to J. Stephenson for informative correspondence, to G. Stell for his generous and instructive discussions, and thanks D. Klinger for informative and clarifying remarks. This work was supported by the National Science Foundation of Switzerland, the National Science Foundation of the United States of America, and the Cornell University Materials Science Center.

1L. S. Ornstein and F. Zernike, Proc. Akad. Sci. (Amsterdam) 17, 793 (1914); reprinted in *Classical Fluids,* edited by H. L. Frisch and J. L. Lebowitz (Benjamin, New York, 1964), p. III-3.

2(a) J. K. Percus, in *Classical Fluids,* (Ref. 1), p. II-33; (b) in *Studies in Statistical Mechanics,* edited by E. W. Montroll and J. L. Lebowitz (North-Holland, Amsterdam, 1982), Vol. VIII, pp. 31–140.

3B. Kaufman and L. Onsager, Phys. Rev. 76, 1244 (1949).

4J. K. Percus, Ref. 2(a).

5J. K. Percus, J. Stat. Phys. 16, 299 (1977).

6J. K. Percus, J. Stat. Phys. 28, 67 (1982).

7J. K. Percus, J. Math. Phys. 23, 1162 (1982).

8G. Stell. Phys. Rev. 184, 135 (1969).

9W. K. Theumann, Phys. Lett. 32A, 1 (1970).

10G. Stell, Physica 29, 517 (1963).

11J. Stephenson, Can. J. Phys. 48, 1724 (1970).

12It may be noted that our result (3.5) for $\hat{h}(q)$ differs from the expression for $\hat{h}(q)$ obtained by Stephenson in his formula (5.6) [Phys. Rev. B 15, 5442 (1977)]. The reason for this difference is due to his choice of the value of $h(0)$. Stephenson apparently calculated $h(0)$ by merely setting $|n|=0$ in his formula (5.1), which is just our formula (2.1) in different notation, getting therefore $h(0)=1$, whereas we have taken $h(0)=-1$, for reasons given above before (3.5).

13See, for example, E. T. Whittaker and G. N. Watson, *A Course in Modern Analysis* (Cambridge University Press, Cambridge, England, 1978), p. 117.

14See, for example, G. H. Hardy, *A Course of Pure Mathematics* (Cambridge University Press, Cambridge, England, 1975), p. 127 and pp. 377–378, Examples LXXVIII, Nos. 2 and 5.

15S. Fisk and B. Widom, J. Chem. Phys. 50, 3219 (1969).

[16]M. Robert and B. Widom (unpublished).

[17]It is not clear whether this property holds in real systems. For example, approximate calculations of the direct correlation function using scattering data for fluid argon apparently suggest that the direct correlation function does not oscillate as strongly, if at all, as the pair correlation function: see P. G. Mikolaj and C. J. Pings, J. Chem. Phys. 46, 1412 (1967).

[18](a) M. S. Green, J. Chem. Phys. 33, 1403 (1960); (b) M. Fisher, J. Math. Phys. 5, 944 (1964).

[19]B. Widom, Science 157, 375 (1967).

[20]See, for example, M. Fisher and B. Widom, J. Chem. Phys. 50, 3756 (1969), Sec. IV.

[21]J. Groeneveld and G. Stell (unpublished). The author is grateful to G. Stell for clarifying comments on this point.

[22]G. Stell, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, London, 1975), Vol. 5B, Chap. 3, Appendix A, Sec. A.3, pp. 252—253.