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Spin-spin correlations in finite systems: Scaling hypothesis and corrections to bulk behavior

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We study the correlation function $G(\mathbf{R},T;L)$ and the correlation length $\xi(T;L)$ in a finite spherical model of size $L^{d-d'}\times\infty^{d'}$ under periodic boundary conditions and emphasize the role of the quantity $L/\xi(L)$, rather than $L/\xi(\infty)$, as the scaled length of the system throughout the transition region, including temperatures below $T_c(\infty)$. We obtain a variety of finite-size effects, some of which may have validity for all $O(n)$ models with $n>2$.

Finite-size scaling theory for critical phenomena, formulated by Fisher[1] almost 15 years ago, has met with considerable success in describing the "rounding of the bulk singularities" in finite systems[2] at temperatures close to $T_c(\infty)$. By contrast, finite-size effects in the region of a first-order phase transition $[T<T_c(\infty)]$ began to be explored only recently. A systematic study of such effects was initiated by Privman and Fisher for both Ising-like models[3] and $O(n)$ models,[4] confined to a "block" (L^d) or a "cylinder" ($L^{d-1}\times\infty^1$) geometry, under periodic boundary conditions. Corroborative studies on the spherical model[5,6] and the ideal Bose gas[7] have also been carried out. In the work of Singh and Pathria,[6,7] the geometry considered has been fairly general, viz., $L^{d-d'}\times\infty^{d'}$, of which the block ($d'=0$) and the cylinder ($d'=1$) are two special cases. In a more recent communication,[8] these authors have shown, in particular, how one may predict the approach of the given system toward standard bulk behavior, as $L\to\infty$, in terms of the bulk exponents pertaining to both d and d' dimensions. Most of this work, however, relates to the thermodynamics of the system, very little attention having been paid to the problem of correlations.[9]

In this paper we present results of the first detailed study of spin-spin correlations in a spherical model of general geometry $L^{d-d'}\times\infty^{d'}$, with $2<d<4$, under periodic boundary conditions. By previous experience,[8] some of these results, especially the ones for the exponents, may be applicable to all $O(n)$ systems with $n>2$. One of the key findings of this study is that the quantity $L/\xi(L)$, where $\xi(L)$ is a *finite-size* correlation length pertaining to the actual system, rather than $L/\xi(\infty)$, where $\xi(\infty)$ is the corresponding *bulk* correlation length, emerges as the natural scaled length of the system. Not only does this vindicate previous assertions[10] as to the role played by the quantity $\xi(L)/L$ in establishing "correspondence between finite systems, similar in shape but different in size" but it also enables us to carry out a detailed study of the temperature dependence of $\xi(L)$ itself in the various regions of interest. At the same time, it provides a basis for probing the system at temperatures below $T_c(\infty)$, where $L/\xi(L)\ll 1$. This could not be possible with the variable $L/\xi(\infty)$, which vanishes identically for $T\leq T_c(\infty)$; see, for instance, Luck.[9] We also derive an explicit expression for the finite-size correction $G^*(\mathbf{R},T;L)$, to the bulk correlation function $G(\mathbf{R},T;\infty)$, which can be studied in detail for various values of R $(=|\mathbf{R}|)$ in relation to the parameters L and $\xi(L)$.

We consider a system of size $L^{d-d'}\times\infty^{d'}$, under periodic boundary conditions, for which the Privman-Fisher hypothesis for the singular part of the free-energy density may be written as[8,11]

$$f^{(s)}(T,H;L)\approx TL^{-d}Y(x_1,x_2)\ , \tag{1}$$

where $x_1=\tilde{C}_1L^{1/\nu}\tilde{t}$, $x_2=\tilde{C}_2L^{\Delta/\nu}H/T$, $\tilde{C}_1$ and $\tilde{C}_2$ are model-dependent scale factors, while $\tilde{t}(T)$ is a generalization of the conventional reduced variable t $\{=[T-T_c(\infty)]/T_c(\infty)\}$ such that $\tilde{t}\to t$ as $T\to T_c(\infty)$; the other symbols have their usual meanings. It is easily seen that a scaling hypothesis for the correlation function, consistent with (1), is

$$G(\mathbf{R},T,H;L)\approx a^{2d}\tilde{C}_2^2R^{2-d-\eta}X(\mathbf{R}/\xi,L/\xi,x_2)\ , \tag{2}$$

where a is a microscopic length, such as the lattice constant, while ξ is a finite-size correlation length obeying the subsidiary hypothesis

$$\xi(T,H;L)\approx LS(x_1,x_2)\ . \tag{3}$$

Following the line of argument adopted in Ref. 8, we predict that, for $T<T_c(\infty)$ and $L\to\infty$, ξ will obey a power law,

$$\xi=D_-L^{(\nu+\dot{\nu})/\nu}|\tilde{t}|^{\dot{\nu}}\ , \tag{4}$$

for $d'<2$, while for $d'=2$ it will diverge exponentially; here, $\dot{\nu}$ denotes the bulk index akin to ν but pertaining to a d'-dimensional system. Moreover, to reproduce the field-free, bulk correlation function (for $r_j\gg a$), namely,[12-14]

$$G(\mathbf{R},T,0;\infty)=M_0^2(T)+A(T)R^{2-d}\ \ [T<T_c(\infty)]\ , \tag{5}$$

where $M_0(T)$ is the spontaneous magnetization and $A(T)$ a system-dependent coefficient, the scaling function X in (2) must possess the asymptotic behavior

$$[X(\mathbf{r},l,0)]_{(r,l)\ll 1}\simeq X_1(rl^{-(\nu+\dot{\nu})/\dot{\nu}})^{2\beta/\nu}+X_2(rl^{-(\nu+\dot{\nu})/\dot{\nu}})^{\eta}+X^*(\mathbf{r},l)\ , \tag{6}$$

with universal amplitudes

$$X_1 = a^{-2d} D_-^{-2\beta/\dot{\nu}} [M_0^2(T) \tilde{C}_2^{-2} |\tilde{t}|^{-2\beta}] , \quad (7)$$

and

$$X_2 = a^{-2d} D_-^{-\nu\eta/\dot{\nu}} [A(T) \tilde{C}_2^{-2} |\tilde{t}|^{-\nu\eta}] , \quad (8)$$

while $X^*(\mathbf{r},l)$ represents the finite-size effect in X. Near $T=T_c(\infty)$, Eqs. (7) and (8) imply that, whereas $M_0(T) \propto |t|^\beta$, $A(T) \propto |t|^{\nu\eta}$—in perfect agreement with Ref. 14. Away from $T_c(\infty)$, they tell us how $\tilde{t}$ and $\tilde{C}_2$ should vary with T:

$$|\tilde{t}| \propto (M_0^2 A^{-1})^{1/(d-2)\nu}; \quad \tilde{C}_2 \propto (M_0^{\gamma-2\nu} A^\beta)^{1/(d-2)\nu} ,$$

in perfect agreement with Ref. 8, where these quantities were determined using the bulk information for $T \gtrsim T_c(\infty)$.

For analytical study we consider a field-free spherical model, of size $L_1 \times \cdots \times L_d$, for which the spin-spin correlation function is given by[13,15]

$$G(\mathbf{R},T;L_j) = \frac{1}{2\beta N} \sum_{\{n_j\}} \frac{\cos(\mathbf{k}\cdot\mathbf{R})}{\lambda - 2J \sum_j \cos(k_j a)} , \quad (9)$$

where $n_j = 0, 1, \ldots, (N_j - 1)$, $N_j = L_j/a$, $k_j = 2\pi n_j/N_j$, while $j = 1, \ldots, d$. Following the methods of Ref. 6, we obtain (for $R_j, L_j >> a$)

$$G(\mathbf{R},T;L_j) = \frac{1}{4\pi K}\left(\frac{\phi}{2\pi}\right)^{(d-2)/2} \sum_{\{q_j\}=-\infty}^{\infty} \frac{K_{(d-2)/2}(\lambda(q_j))}{[\lambda(q_j)]^{(d-2)/2}} , \quad (10)$$

where $K = \beta J, K_\nu(z)$ are the modified Bessel functions,

$$\lambda(q_j) = \frac{\sqrt{\phi}}{a}\left(\sum_{j=1}^{d} (q_j L_j + R_j)^2\right)^{1/2} , \quad \phi = \left(\frac{\lambda}{J} - 2d\right) << 1 ; \quad (11)$$

the parameter $\phi(T;L_j)$ is determined by the constraint equation

$$8\pi(K_c - K) = \left(\frac{\phi}{4\pi}\right)^{(d-2)/2} \left[\left|\Gamma\left(\frac{2-d}{2}\right)\right| - 2^{d/2} \sum_{q \neq 0} \frac{K_{(d-2)/2}(\lambda_0(q_j))}{[\lambda_0(q_j)]^{(d-2)/2}}\right] , \quad (12)$$

where λ_0 denotes $(\lambda)_{\mathbf{R}=0}$. Recalling our expressions for $\tilde{t}$, $\tilde{C}_1$, and $\tilde{C}_2$ for the spherical model,[8] we readily see that, for geometry $L^{d-d'} \times \infty^{d'}$, Eqs. (10)–(12) conform to the scaling hypothesis (2), with

$$\xi(T;L) = a/\sqrt{\phi(T;L)} = L/2y(x_1) , \quad (13)$$

y being the *thermogeometric parameter*[6] of the system. At the same time, Eq. (13) conforms to the subsidiary hypothesis (3), with

$$S(x_1, 0) = 1/2y(x_1) . \quad (14)$$

From the known behavior of y, we can now show that, for $\tilde{t} > 0$ and $L \to \infty$,

$$\delta(\xi) = \frac{\xi(L) - \xi(\infty)}{\xi(\infty)} \simeq -\left[d^* \pi^{1/2} \Big/ \Gamma\left(\frac{4-d}{2}\right)\right] \left(\frac{2\xi(\infty)}{L}\right)^{(d-1)/2} e^{-L/\xi(\infty)} , \quad (15)$$

where $\xi(\infty) \sim a\tilde{t}^{-\nu}$, while $d^* = d - d'$; this generalizes a recent result of Luck[9] which pertained to the special case $d'=1$. In the close vicinity of $T_c(\infty)$, $\xi(L) = O(L)$ and its precise value can be obtained only numerically; for the exceptional cases $d \gtrsim 2$ and $d \lesssim 4$, however, we obtain the following analytical results:

$$2\pi^{1/2}\left(\frac{\xi(L)}{L}\right)_c \simeq \begin{cases} [\frac{1}{2}\Gamma((2-d')/2)\epsilon]^{-1/(2-d')} & (\epsilon = d-2 << 1) , \\ [\frac{1}{2}\Gamma((2-d')/2)\epsilon]^{-1/(4-d')} & (\epsilon = 4-d << 1) , \end{cases}$$

where $d' < 2$. This generalizes certain other results of Luck[9] (valid for $d'=1$) and some of Brézin[9] (valid for $d'=0$ and 1). For $\tilde{t} < 0$ and $L \to \infty$, we find that prediction (4) is verified. Accordingly, for $d' < 2$,

$$\xi \propto L^{(d-d')/(2-d')} |\tilde{t}|^{1/(2-d')} \quad (16)$$

and the amplitude D_- is determined; for $d'=2$, on the other hand, ξ diverges as $L \exp(4\pi \tilde{C}_1 L^{d-2} |\tilde{t}|)$.

As for the correlation function $G(\mathbf{R},T;L)$, it satisfies all the requirements stipulated in Eqs. (6)–(8). While details will be published elsewhere, we summarize some of the more important results here. First of all, for $R << \xi$, the correlation function assumes the remarkable form, cf. Eqs. (5) and (6),

$$G(\mathbf{R},T;L) = \left(1 - \frac{K_c}{K}\right) + \frac{\Gamma((d-2)/2)}{8\pi^{d/2} K}\left(\frac{a}{R}\right)^{d-2} + G^*(\mathbf{R},T;L) , \quad (17)$$

where

$$G^*(\mathbf{R},T;L) = \frac{1}{4\pi K}\left(\frac{\phi}{2\pi}\right)^{(d-2)/2} \sum_{q(d^*)}{}' \left(\frac{K_{(d-2)/2}(\lambda(\mathbf{q}))}{[\lambda(\mathbf{q})]^{(d-2)/2}} - \frac{K_{(d-2)/2}(\lambda_0(\mathbf{q}))}{[\lambda_0(\mathbf{q})]^{(d-2)/2}}\right) , \quad (18)$$

$$\lambda(\mathbf{q}) = \frac{1}{\xi}\left(\sum_{j=1}^{d^*} (q_j L + R_j)^2 + R_\parallel^2\right)^{1/2} , \quad R_\parallel^2 = R^2 - R_\perp^2 , \quad R_\perp^2 = \sum_{j=1}^{d^*} R_j^2 , \quad (19)$$

while the primed summation in (18) implies that the term with $\mathbf{q}(d^*)=0$ is excluded. The foregoing result is consistent with the expectation[12] that

$$\lim_{R\to\infty}\Big[\lim_{L_j\to\infty} G(\mathbf{R},T;L_j)\Big]=M_0^2(T) \quad . \tag{20}$$

Expression (18) leads to a variety of finite-size effects. In particular, for $T < T_c(\infty)$ and $L \to \infty$, we obtain a much simpler result:

$$G^*(\mathbf{R},T;L)=\frac{\Gamma((d-2)/2)}{8\pi^{d/2}K}\left(\frac{a}{L}\right)^{d-2}\sum_{\mathbf{q}(d^*)}{}^{'}\left\{\left[\left(\mathbf{q}+\frac{\mathbf{R}_\perp}{L}\right)^2+\left(\frac{R_\parallel}{L}\right)^2\right]^{-(d-2)/2}-q^{-(d-2)}\right\} \quad . \tag{21}$$

Further simplification results if $R \ll L$; we get

$$G^*(\mathbf{R},T;L)=\begin{cases}\dfrac{\Gamma(d/2)}{8\pi^{d/2}d^*K}\left(\displaystyle\sum_{\mathbf{q}(d^*)}{}^{'}q^{-d}\right)\left(\dfrac{a}{L}\right)^{d-2}\left(d'\dfrac{R_\perp^2}{L^2}-d^*\dfrac{R_\parallel^2}{L^2}\right) & (0<d'\leq 2) \;, \\[2ex] \dfrac{1}{4dK}\left(\dfrac{a}{L}\right)^{d-2}\left(\dfrac{R}{L}\right)^2 & (d'=0) \;. \end{cases}$$

If R is not $\ll L$ and/or L is not $\ll \xi$, then series expansions can be carried out in the manner Zasada and Pathria did for the Bose gas;[9] explicit results have thus been obtained for the most practical cases (namely, $d=3$ and $d'=0$, 1, and 2), and will be reported subsequently.

For $R \gg L$, which implies that $R_\parallel \gg L$, we can no longer talk of a finite-size *correction* to the bulk correlation function; we have instead a qualitatively different situation. To see this, we transform (10) into the form

$$G(\mathbf{R},T;L)=\frac{1}{4\pi^{d'/2}K}\left(\frac{a}{L}\right)^{d-2}\left(\frac{R_\parallel}{L}\right)^{(2-d')/2}\sum_{\mathbf{n}(d^*)}\frac{\cos[2\pi(\mathbf{n}\cdot\mathbf{R}_\perp)/L]K_{(2-d')/2}(2(n^2\pi^2+y^2)^{1/2}R_\parallel/L)}{(n^2\pi^2+y^2)^{(2-d')/4}} \quad , \tag{22}$$

and note that, for $R_\parallel \gg L$, the most dominant contribution to the sum comes from the term with $\mathbf{n}=0$, with the result that

$$G_{d,d^*}(\mathbf{R},T;L)\simeq(a/L)^{d^*}G_{d',0}(R_\parallel,T) \quad . \tag{23}$$

Thus, the correlation function essentially splits into two factors—one pertaining to the finite dimensions of the system and the other pertaining to the infinite ones; of course, the correlation length entering into the latter will still pertain to the actual system. While this last result is highly suggestive, full implications of (22) cannot be realized unless the contribution of terms with $\mathbf{n}\neq 0$ is properly assessed. Work in that direction is in progress.

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