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Finite-Size Shift of the Critical Temperature in the Spherical Model

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The finite-size shift of the critical temperature is calculated by the example of the spherical model, with short- and long-range interactions, confined to the general geometry $L^{d-d'} \times \infty^{d'}$ subject to periodic boundary conditions. The derived formula unifies in some sense all results found up to now.

KEY WORDS: Spherical model; finite-size shift; long-range interaction.

1. INTRODUCTION

Thermodynamic functions exhibit singularities at a point of second-order phase transition in the thermodynamic limit only, i.e., when the number of the particles N and the volume V of the system are infinite. However, if some sizes of the system are finite, the thermodynamic properties of the system are altered (for details see ref. 1 and references therein).

According to finite-size scaling theory, a phase transition occurring in a system at the thermodynamic limit persists if the dimension d' of infinite sizes is greater than the lower critical dimension $d_<$ of the system. In this case the value of the critical temperature $T_c(\infty)$ at which some thermodynamic functions exhibit a singularity is shifted to $T_c(L^{d-d'} \times \infty^{d'}; d' > d_<)$, the critical temperature for a system confined to the general geometry $L^{d-d'} \times \infty^{d'}$; when the system is infinite in d' dimensions and finite in $d-d'$ dimensions. In the other case, i.e., when the number of infinite dimensions is less than the lower critical dimension, there is no phase transition in the system and the singularities of the thermodynamic functions are rounded and shifted. The critical temperature $T_c(\infty)$ in this case is shifted to a pseudocritical temperature $T_c(L^{d-d'} \times \infty^{d'}; d' < d_<)$,

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corresponding to the center of the rounding of the singularities of the thermodynamic functions, holding in the thermodynamic limit.

The aim of the present note is to evaluate the distance over which the critical temperature $T_c(\infty)$ of the bulk system is shifted in a finite system, by the example of the spherical model with interaction decaying at large distances r as $r^{-d-\sigma}$, where σ is a parameter determining the range of the interactions: (i) $0<\sigma<2$ for long-range interaction and (ii) $\sigma \geqslant 2$ for short-range interaction. We suppose that the finite system is confined to the geometry $L^{d-d'} \times \infty^{d'}$ and that the boundary conditions are periodic.

The problem of the evaluation of the shift of the critical temperature for the bulk system and related finite-size effects has been investigated by several authors.[2-7] For the spherical model various techniques have been used to evaluate the shift: (i) When there is no phase transition in the system a formula for the finite-size shift (for the fully finite system with short-range interaction in particular for $\sigma=2$) has been derived by Shapiro and Rudnick[4] using an approach based on numerical approximations, (ii) for the same case but in a system with long-range and short-range interaction ($0<\sigma \leqslant 2$) the shift has been found by Brankov and Tonchev,[5] and (iii) for the case when the system exhibits a phase transition the finite-size shift has been calculated by Brézin[3] (for $d'=d-1$) and Allen and Pathria[6] (for $d_< < d' < d_>$, where $d_>$ is the upper critical dimension). These results consider that the interaction in the system is of short range. Brankov and Danchev[7] derived the following formula for a system with long-range interaction and $d_< = \sigma < d' < d_> = 2\sigma$:

$$\frac{1}{T_c(L^{d-d'} \times \infty^{d'};\, d' > d_<)} - \frac{1}{T_c(\infty)} = \frac{1}{\rho_\sigma} \frac{\Gamma(d/2-\sigma/2)}{(4\pi)^{d/2}\, \Gamma(\sigma/2)} \sum_{l(d-d')}{}' \left(\frac{|l|\, L}{2}\right)^{-d+\sigma} \tag{1.1}$$

where $l(d-d')$ means that the summation is over $l \in Z^{d-d'}$, and the prime denotes that the term with $l=0$ is excluded. For the meaning of the parameter ρ_σ see below.

Formula (1.1) generalizes the above results of Brézin and of Allen and Pathria.

In this note we find a formula which unifies all the results obtained for the finite-size shift for the spherical model.

2. GENERAL FORMULA

For the sake of completeness in this section we will introduce some concepts and notations which will be useful later. The Hamiltonian of the model is defined on a d-dimensional lattice $\mathscr{L} = L_1 \times L_2 \times \cdots \times L_d$ subject to periodic boundary conditions. The Fourier transform of the effective potential

$$\mathscr{T}(\mathbf{q}) = \sum_{l \in \mathscr{L}} \tilde{\mathscr{T}}_{\mathscr{L}}(l) \exp(-i l \cdot \mathbf{q}) \tag{2.1}$$

has the following long-wavelength asymptotic behavior ($\rho_\sigma > 0$):

$$\mathscr{T}(\mathbf{q}) \approx \mathscr{T}(0)(1 - \rho_\sigma |\mathbf{q}|^\sigma), \qquad |\mathbf{q}| \to 0 \tag{2.2}$$

The mean spherical constraint has the form

$$1 = t \mathscr{W}^L_{d,\sigma}(\tilde{\phi}) \equiv \frac{t}{N} \sum_{\mathbf{q}} (\tilde{\phi} + |\mathbf{q}|^\sigma)^{-1} \tag{2.3}$$

where the parameters are $t = T/\rho_\sigma$ and $\tilde{\phi} = \phi/\rho_\sigma$ ($\phi = 2s/\mathscr{K} - 1$ is a linear function of the spherical field s).

When the spherical model is confined to the general geometry $L^{d-d'} \times \infty^{d'}$, the asymptotic behavior of the sum in the right-hand side of the spherical constraint (2.3) takes the form[9]

$$\mathscr{W}^L_{d,d',\sigma}(\tilde{\phi}) = \mathscr{W}_{d,\sigma}(\tilde{\phi}) + \delta \mathscr{W}^L_{d,d',\sigma}(\tilde{\phi}) \tag{2.4}$$

where

$$\mathscr{W}_{d,\sigma}(\tilde{\phi}) = (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\mathbf{q} (\tilde{\phi} + |\mathbf{q}|^\sigma)^{-1} \tag{2.5}$$

is the bulk contribution and

$$\delta \mathscr{W}^L_{d,d',\sigma}(\tilde{\phi}) = \frac{L^{\sigma-d}}{(4\pi)^{d/2}} \sum_{l(d-d')}{}' \int_0^\infty dx \exp\left(-\frac{|l|^2}{4x}\right) \times x^{\sigma/2 - d/2 - 1} E_{\sigma/2,\sigma/2}(-x^{\sigma/2} L^\sigma \tilde{\phi}) \tag{2.6}$$

is the finite-size correction. In Eq. (2.6) the function

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)} \tag{2.7}$$

is the so called Mittag–Leffler function.

The asymptotic form of expression (2.4) in the large-L limit can be found using the method suggested in ref. 5. This method has been used to find the asymptotic form of the equation for the mean-spherical field for the fully finite system $d'=0$. A straightforward generalization of this method is possible for a system confined to the general geometry $L^{d-d'}\times\infty^{d'}$. After some algebra we obtain

$$\delta \mathscr{W}^{L}_{d,d',\sigma}(\tilde{\phi}) = L^{\sigma-d}(L^{\sigma}\tilde{\phi})^{d'/\sigma-1}D_{d',\sigma} - \tilde{\phi}^{d/\sigma-1}D_{d,\sigma} + C_{d,d',\sigma}(\tilde{\phi}) + \frac{L^{\sigma-d}}{(2\pi)^{\sigma}}\frac{\pi^{d'/2}}{\Gamma(\sigma/2)}\mathscr{E}_{d,d',\sigma} \tag{2.8}$$

where we introduce the notations

$$D_{d,\sigma} = \frac{1}{(4\pi)^{d/2}}\int_0^{\infty} dx\, x^{\sigma/2-d/2-1}E_{\sigma/2,\sigma/2}(-x^{\sigma/2}) \tag{2.9}$$

$$C_{d,d',\sigma}(\tilde{\phi}) = \frac{L^{\sigma-d}}{2^{\sigma}\pi^{(\sigma-d'/2)}}\sum_{l(d-d')}{}' \int_0^{\infty} dx\, x^{\sigma/2-d'/2-1}\exp(-x\,|l|^2) \times\left[E_{\sigma/2,\sigma/2}\left(-\frac{x^{\sigma/2}L^{\sigma}\tilde{\phi}}{(2\pi)^{\sigma}}\right)-\frac{1}{\Gamma(\sigma/2)}\right] \tag{2.10}$$

$$\begin{aligned}\mathscr{E}_{d,d',\sigma} &= \sum_{l(d-d')}{}' \int_0^{\infty} dx\, x^{\sigma/2-d'/2-1}\exp(-x\,|l|^2) - \pi^{(d-d')/2}\int_0^{\infty} dx\, x^{\sigma/2-d/2-1}\\ &\equiv \lim_{\lambda\to 0}\left\{\sum_{l(d^*)}\Gamma(\sigma^*/2,\lambda l^2)\,|l|^{-\sigma^*} - \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} d^d l\,\Gamma(\sigma^*/2,\lambda l^2)\,|l|^{-\sigma^*}\right\}\end{aligned} \tag{2.11}$$

Here $d^*=d-d'$, $\sigma^*=\sigma-d'$, and $\Gamma(\alpha,x)$ is the incomplete gamma function. From (2.11) one can see that $\mathscr{E}_{d,d',\sigma}$ is a generalization of the Madelung-type constant.[5]

From Eqs. (2.3), (2.4), and (2.8), we write down the equation of the spherical field in the form

$$\frac{1}{t} = \mathscr{W}_{d,\sigma}(\tilde{\phi}) + L^{\sigma-d}(L^{\sigma}\tilde{\phi})^{d'/\sigma-1}\,D_{d',\sigma} - \tilde{\phi}^{d/\sigma-1}D_{d,\sigma} + C_{d,d',\sigma}(\tilde{\phi}) + \frac{L^{\sigma-d}}{(2\pi)^{\sigma}}\frac{\pi^{d'/2}}{\Gamma(\sigma/2)}\mathscr{E}_{d,d',\sigma} \tag{2.12}$$

The next step consist in the evaluation of the finite-size shift of the critical temperature, generalizing the result of ref. 5. It is

$$\frac{1}{t_c(L^{d-d'}\times\infty^{d'};\, d'\neq d_<)}-\frac{1}{t_c(\infty)}=\frac{L^{\sigma-d}}{(2\pi)^{\sigma}}\frac{\pi^{d'/2}}{\Gamma(\sigma/2)}\mathscr{E}_{d,d',\sigma} \tag{2.13}$$

The notation $T_c(L^{d-d'}\times\infty^{d'};\, d'\neq d_<)$ in Eq. (2.13) is the finite-size pseudocritical temperature for $d'<\sigma$ and the finite-size critical temperature for $d'>\sigma$. Notice that for $d'=0$ we refined the formula derived in ref. 5.

Because the bulk critical exponent ν_d measuring the divergence of the correlation length ξ of the d-dimensional system is equal to $1/(d-\sigma)$ for $\sigma<d<2\sigma$ and to $1/\sigma$ for $d>2\sigma$, we see from Eq. (2.13) that the L dependence of the finite-size shift of the critical temperature is L^{-1/ν_d} in the former case and smaller than L^{-1/ν_d} in the latter. This is in agreement with the finite-size scaling prediction; see, e.g., the result for the short-range case $(\sigma=2)$ due to Brézin.[3]

3. CONCLUSION

We will show that the two formulas (1.1) and (2.13) found for the finite-size shift of the critical temperature are equivalent for some d' and σ.

Using the notations $m=d-d'$ and $\nu=(d-\sigma)/2$ in the r.h.s. of Eq. (2.11), we refined the r.h.s. of Eq. (A1.1) of ref. 10 for $\lambda=0$. According to this equation, we have

$$\mathscr{E}_{d,d',\sigma}=\frac{\Gamma(d/2-\sigma/2)}{\pi^{d/2-d'/2-\sigma}}\sum_{l(d-d')}{}' \, |l|^{-d+\sigma} \tag{3.1}$$

and from Eqs. (2.13) and (3.1) we recover the formula (1.1). The proof of the identity (3.1) is, however, limited to the case when $\nu>m/2$. In our notations this corresponds to the case when $d'>\sigma$.

The sum in the r.h.s. of Eq. (3.1) can be expressed in terms of the Epstein zeta function[11]

$$\mathscr{Z}\begin{vmatrix}0\\0\end{vmatrix}(d-d', d-\sigma)=\sum_{l(d-d')}{}' \frac{1}{|l|^{d-\sigma}} \tag{3.2}$$

which can be regarded as the generalized $(d-d')$-dimensional analog of the Riemann zeta function $\zeta(d/2-\sigma/2)$. In the case under consideration the Epstein zeta function has only a simple pole at $d'=d_<$ and may be analytically continued for $0\leqslant d'<d_<$. For some particular values of the finite dimensions of the lattice this sum may be expressed as a product of simple sums such as Dirichlet series. This is done for $d^*=1$, 2, 4, 6, and 8 in

Table I. Shift of the Critical Temperature for Typical Values of the Space Dimensionality

	$\delta t\, L^{d-\sigma}$			
	$d=2$		$d=3$	
d'	$\sigma=1/2$	$\sigma=1$	$\sigma=1$	$\sigma=2$
0	-0.766643	-0.620746	-0.800387	-0.225785
1	0.397469	$\mp\infty$	$\mp\infty$	-0.310373
2	0	0	0.166667	$\mp\infty$
3	—	—	0	0

ref. 10. The more interesting 3D case has been investigated numerically by Glasser and Zucker.[11]

The behavior of $\delta t\, L^{d-\sigma}$ as a function of σ and some numerical results in the most interesting cases are presented in Table I and Figs. 1–4.

The result for $d=3$, $d'=0$, and $\sigma=2$ was obtained in ref. 5. One can see that the shifted critical temperature $T_c(L^{d-d'} \times \infty^{d'};\ d' > d_<)$ is lower than the critical bulk critical temperature $T_c(\infty)$ for the different values of d, d', and σ (which is the "normal case"; see ref. 3), while the pseudocritical $T_c(L^{d-d'} \times \infty^{d'};\ d' < d_<)$ is greater than the bulk critical temperature. However, for the boundary case when $d' \to d_<$ we find that the shift is infinite. This may be explained with the aid of the behavior of the Epstein zeta function at its pole $d' = \sigma$.[11] The shift in this case is $\delta t \sim (d' - \sigma)^{-1}$ and the appearance of $\mp\infty$ is clear.

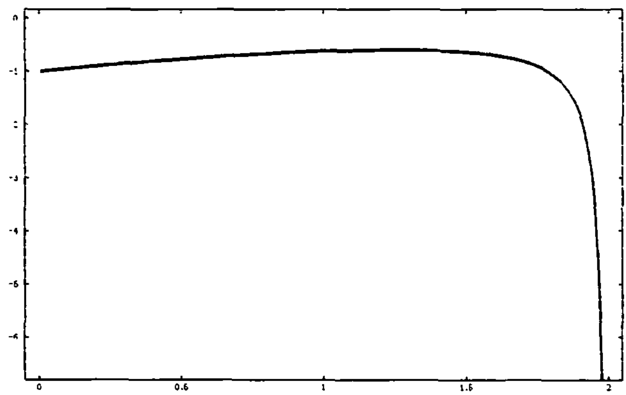

Fig. 1. The shift of the critical temperature as a function of σ for $d=2$ and $d'=0$.

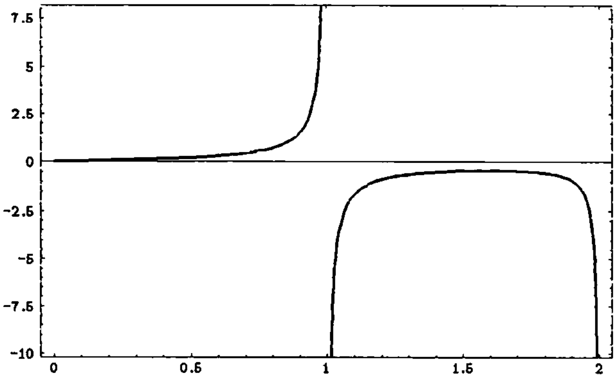

Fig. 2. The shift of the critical temperature as a function of σ for $d=2$ and $d'=1$.

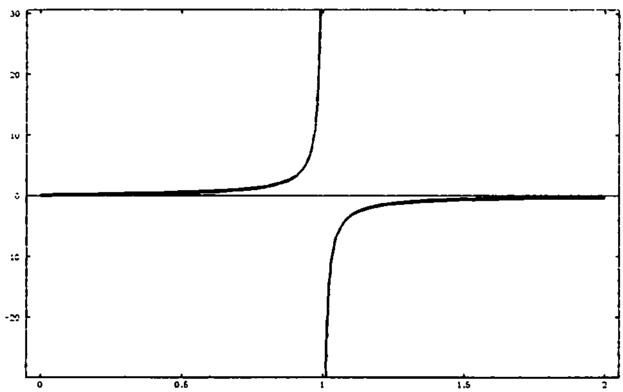

Fig. 3. The shift of the critical temperature as a function of σ for $d=3$ and $d'=1$.

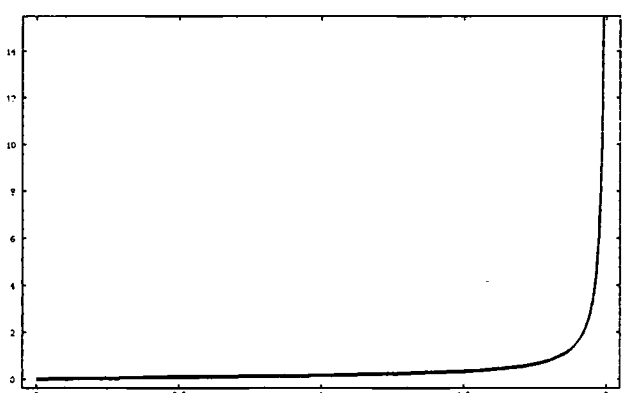

Fig. 4. The shift of the critical temperature as a function of σ for $d=3$ and $d'=2$.

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