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CRITICAL CASIMIR FORCE SCALING FUNCTIONS OF THE MEAN SPHERICAL MODEL IN $2<d\leq 3$ DIMENSIONS FOR NONPERIODIC BOUNDARY CONDITIONS

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Finite-size effects are investigated in the mean spherical model in film geometry with nonperiodic boundary conditions above and below bulk T_c. We have obtained exact results for the excess free energy and the Casimir force for antiperiodic, Neumann, Dirichlet, and Neumann-Dirichlet mixed boundary conditions in $2 < d \leq 3$ dimensions. Analytic results are presented in $2 < d < 3$ dimensions for Dirichlet boundary conditions and for $d = 3$ for Neumann-Dirichlet boundary conditions. We find an unexpected leading size dependence $\propto C_\pm t/L^2$ of the Casimir force, with different amplitudes C_+ and C_- above and below T_c for large L at fixed $t \equiv (T - T_c)/T_c \neq 0$ for other than periodic boundary conditions.

Keywords: Mean spherical model; Exact solution; Free energy; Critical Casimir force; Finite-size scaling; Scaling function.

1. Introduction

Little is known about finite-size effects of critical systems below the bulk transition temperature T_c for realistic boundary conditions, such as Dirichlet or Neumann boundary conditions. Even for the exactly solvable mean spherical model[1,2] no finite-size investigation has been performed so far below T_c for nonperiodic boundary conditions. Previous studies of this model for the case of Dirichlet (or free) boundary conditions for $T \geq T_c$ have shown that finite-size scaling is violated in $d = 3$ dimensions[1,2] whereas finite-size scaling holds in $2 < d < 3$ dimensions.[2] Here we present exact results of the free energy and the Casimir force of this model above and below bulk T_c in film geometry with various nonperiodic boundary conditions in $2 < d \leq 3$ dimensions. The validity of finite-size scaling below three dimensions is confirmed and the Casimir force finite-size scaling functions for nonperiodic boundary conditions in $d = 2.5$ dimensions are graphically displayed. As unexpected results we find the validity of finite-size scaling in $d = 3$ dimensions for mixed Neumann-Dirichlet boundary conditions and a leading size dependence $\propto C_\pm t/L^2$ of the Casimir force, with different amplitudes C_+ and C_- above and below T_c, for large L at fixed $t \equiv (T - T_c)/T_c \neq 0$ for other than periodic boundary conditions.

2. Model

Consider a d-dimensional simple cubic lattice with lattice spacing a, $\mathcal{N} \equiv \tilde{N}^{d-1} \times N$ sites and volume $V = \tilde{L}^{d-1}L$, where $\tilde{L} \equiv \tilde{N}a$ and $L \equiv Na$. The Hamiltonian of the mean spherical model on this lattice is

$$\mathcal{H} = a^d \left[\frac{J}{2a^2} \sum_{\langle \boldsymbol{x},\boldsymbol{x}' \rangle} (S_{\boldsymbol{x}} - S_{\boldsymbol{x}'})^2 + \frac{\mu}{2} \sum_{\boldsymbol{x}} S_{\boldsymbol{x}}^2 \right], \tag{1}$$

with $J > 0$ and where $\sum_{\langle \boldsymbol{x},\boldsymbol{x}' \rangle}$ denotes a double sum over both primed an unprimed coordinates, where only nearest neighbors ($|\boldsymbol{x} - \boldsymbol{x}'| = a$) contribute. The fluctuations of the scalar spin variables $S_{\boldsymbol{x}}$ are subject to the constraint

$$a^{d-2} \sum_{\boldsymbol{x}} \langle S_{\boldsymbol{x}}^2 \rangle = \mathcal{N}, \tag{2}$$

implying that the "spherical field" μ is not an independent quantity but is a function of $\beta = 1/(k_B T)$ and of the geometry of the system.

As we are only interested in the film limit $\tilde{N} \to \infty$, we only need to specify the boundary conditions in the dth direction. After adding two fictitious sites x_0 and x_{N+1} in the negative and positive dth direction for each value of the remaining $d-1$ coordinates (which we omit from the notation now), the various boundary conditions considered here are defined by

$$\begin{aligned}
&\mathrm{p}: \text{ periodic}, && S_{x_{N+1}} = S_{x_1}, && && (3a)\\
&\mathrm{a}: \text{ antiperiodic}, && S_{x_{N+1}} = -S_{x_1}, && && (3b)\\
&\mathrm{NN}: \text{ Neumann-Neumann}, && S_{x_0} = S_{x_1}, && S_{x_{N+1}} = S_{x_N}, && (3c)\\
&\mathrm{ND}: \text{ Neumann-Dirichlet}, && S_{x_0} = S_{x_1}, && S_{x_{N+1}} = 0, && (3d)\\
&\mathrm{DD}: \text{ Dirichlet-Dirichlet}, && S_{x_0} = 0, && S_{x_{N+1}} = 0, && (3e)
\end{aligned}$$

the terminology being in analogy to the corresponding continuum model.

The dimensionless partition function Z and thermodynamic potential Φ are defined by

$$Z(T,\mu,L,\tilde{L}) = \exp[-\beta\Phi(T,\mu,L,\tilde{L})] = \prod_{x} \int_{-\infty}^{+\infty} \frac{dS_x}{a^{(2-d)/2}} \exp(-\beta\mathcal{H}). \quad (4)$$

The appropriate (Legendre transformed) reduced free-energy density is

$$f(t,L) = \lim_{\tilde{L}\to\infty} \frac{\beta}{\tilde{L}^{d-1}L} \left[\Phi - \mu\left(\frac{\phi\Phi}{\phi\mu}\right)_{T,L,\tilde{L}}\right], \quad (5)$$

with $\mu(t,L)$ determined by the constraint (2) for $\tilde{N}\to\infty$. For $2<d\leq 3$ dimensions there is no phase transition at finite temperature for finite L, but there is a transition at a finite T_c in the bulk limit $L\to\infty$.

The excess free-energy density is $f^{\rm ex}(t,L) = f(t,L) - f(t,\infty)$. We are interested in the thermodynamic Casimir force per unit area[3]

$$F(t,L) = -\frac{\partial[Lf^{\rm ex}(t,L)]}{\partial L}. \quad (6)$$

It is expected[3,4] that $f^{\rm ex}(t,L)$ and $F(t,L)$ can be decomposed into singular and regular parts, $f^{\rm ex} = f^{\rm ex}_{\rm sing} + f^{\rm ex}_{\rm reg}$ and $F = F_{\rm sing} + F_{\rm reg}$. If finite-size scaling holds, the singular parts have the asymptotic (large L, small $|t|$) scaling structure[3,4]

$$f^{\rm ex}_{\rm sing}(t,L) = L^{-d}\mathcal{F}(s), \qquad F_{\rm sing}(t,L) = L^{-d}X(s), \quad (7)$$

with the scaling variable $s = t(L/\xi_0)^{1/\nu}$, $\nu = 1/(d-2)$. The nonuniversal reference length ξ_0 can be chosen as the asymptotic amplitude of the second-moment bulk correlation length $\xi = \xi_0 t^{-\nu}$ above T_c. In the presence of surface contributions it is appropriate to further decompose, for $|t|\neq 0$,

$$f^{\rm ex}_{\rm sing}(t,L) = f^{a}_{\rm surf,sing}(t)L^{-1} + f^{b}_{\rm surf,sing}(t)L^{-1} + L^{-d}\mathcal{G}(s), \quad (8)$$

where a and b denote the two surfaces of the film. The scaling function $X(s)$ is determined by $\mathcal{F}(s)$ and $\mathcal{G}(s)$ according to

$$\begin{aligned} X(s) &= (d-1)\mathcal{F}(s) - (d-2)s\mathcal{F}'(s) \\ &= (d-1)\mathcal{G}(s) - (d-2)s\mathcal{G}'(s). \end{aligned} \quad (9)$$

3. Results

As a cross check, we have successfully compared our expressions for the free energy for periodic boundary conditions with Ref. 5 for $d=3$ and with Ref. 6 for $2<d<3$. As an example with nonperiodic boundary conditions, we provide here the exact result for $X(s)$ for Dirichlet-Dirichlet boundary conditions for $2 < d < 3$,

$$X(s) = -\frac{\Gamma(\frac{2-d}{2})}{2(4\pi)^{d/2}}\left[y_L^2 - \pi^2 - y_\infty^2\right]s - \frac{(d-1)\Gamma(\frac{-d}{2})}{2(4\pi)^{d/2}}\left[y_L^d - y_\infty^d\right]$$
$$-\frac{\Gamma(\frac{3-d}{2})}{2(4\pi)^{(d-1)/2}}y_L^{d-1} - \frac{\pi^2(d-1)\Gamma(\frac{2-d}{2})}{2(4\pi)^{d/2}}y_L^{d-2}$$
$$-\frac{d-1}{2^{d+1}\pi}\int_0^\infty dz\left(\frac{\pi}{z}\right)^{(d+1)/2}e^{-zy_L^2/\pi^2}\left\{e^z[K(z)-1]-\sqrt{\frac{\pi}{z}}+1-\sqrt{\pi z}\right\}, \tag{10}$$

with $y_\infty(s)$ defined by

$$y_\infty \equiv \begin{cases} s^{1/(d-2)} & s > 0, \\ 0 & s \leq 0, \end{cases} \tag{11}$$

and with $y_L(s)$ determined by the constraint, which now reads

$$\Gamma(\tfrac{2-d}{2})(y_L^{d-2} - s) = \sqrt{\pi}\Gamma(\tfrac{3-d}{2})y_L^{d-3} - 2(4\pi)^{d/2}\mathcal{E}_d(y_L), \tag{12}$$

where

$$\mathcal{E}_d(y_L) \equiv \frac{1}{2^{d+1}\pi^2}\int_0^\infty dz\left(\frac{\pi}{z}\right)^{(d-1)/2}e^{-zy_L^2/\pi^2}\left\{e^z[K(z)-1]-\sqrt{\frac{\pi}{z}}+1\right\}, \tag{13}$$

and $K(z) \equiv \sum_{n=-\infty}^{\infty} e^{-n^2 z}$. Similar expressions result for the other boundary conditions of Eq. (3). The $d = 2.5$ results are displayed in Figs. 1(a)-(e) for all these boundary conditions.

For $d = 3$, both the reduced free-energy density and the Casimir force exhibit scaling violations for Neumann-Neumann and Dirichlet-Dirichlet boundary conditions, for example in the form of a logarithmic dependence on L/a at bulk T_c, as will be detailed elsewhere. We find, however, that scaling holds not only for periodic and antiperiodic, but also for mixed Neumann-Dirichlet boundary conditions in three dimensions. The reason for this unexpected behavior will be discussed elsewhere. The Casimir force scaling function for Neumann-Dirichlet boundary conditions reads

$$X_3(s) = -\frac{1}{4}E_3\bar{y}_L^2 + \frac{1}{8\pi}\left(\bar{y}_L^2 - y_\infty^2\right)s - \frac{1}{6\pi}\left(\bar{y}_L^3 - y_\infty^3\right)$$
$$-\frac{1}{8\pi}\left[\mathrm{Li}_3(-e^{-2\bar{y}_L}) + 2\bar{y}_L\mathrm{Li}_2(-e^{-2\bar{y}_L})\right], \tag{14}$$

where Li_2 and Li_3 are polylogarithms, with

$$E_3 \equiv \int_0^\infty dy B(y)^2\left[e^{-2y} - B(y)\right] \approx -0.237167, \tag{15}$$

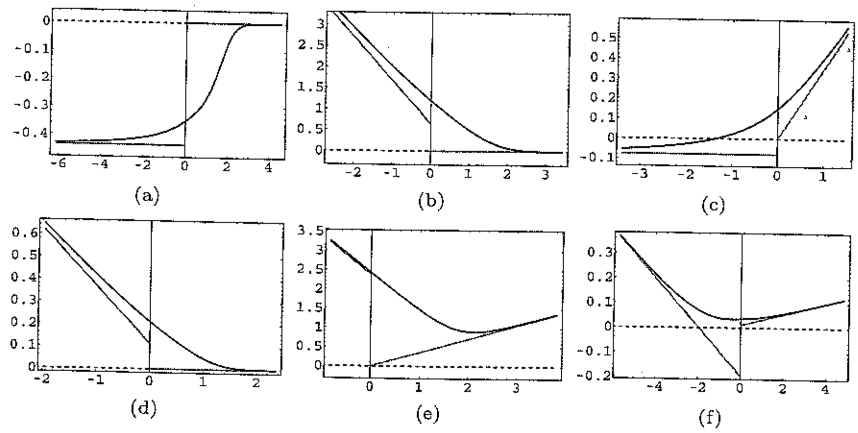

Fig. 1. (a)-(e): Scaling function $X(s)$ of the Casimir force for periodic (a), antiperiodic (b), Neumann-Neumann, (c), Neumann-Dirichlet (d), and Dirichlet-Dirichlet (e) boundary conditions for $d = 2.5$. The grey lines specify the asymptotic ($s \to \pm\infty$) behavior. (f): $X_3(s)$ for Neumann-Dirichlet boundary conditions for $d = 3$.

$y_\infty(s)$ from (11) and $\bar{y}_L(s)$ given by the constraint

$$\bar{y}_L \equiv \sqrt{y_L^2 - \tfrac{\pi^2}{4}} = \operatorname{arcosh}\left(\tfrac{1}{2}e^{s-\pi E_3}\right) \qquad (16)$$

for $y_L \geq \pi/2$ and appropriate analytic continuations to $0 < y_L < \pi/2$. $X_3(s)$ is shown in Fig. 1(f). $X_3(s)$ exhibits a linear asymptotic behavior not only for large negative s [as for $d = 2.5$, see Fig. 1(d)], but also for large positive s.

For other than periodic boundary conditions we find at fixed $|t| \neq 0$ for sufficiently large L that the Casimir force has the leading behavior $F \sim C_\pm t/L^2$ with different amplitudes C_+ and C_- above and below T_c, respectively. In Eqs. (10) and (14) we have included these terms in the singular part F_{sing} which then implies the linear asymptotic behavior of the scaling functions shown in Fig. 1(b)-(f) for large positive and/or negative s for the various nonperiodic boundary conditions. We note here, however, that this unexpected behavior cannot uniquely be attributed to the scaling functions because of an ambiguity in defining the regular part of the Casimir force, as will be discussed elsewhere.

Finally, a reservation must be made with regard to the exponential tails of the L-dependence of the Casimir force. As pointed out elsewhere,[6,7] these tails violate finite-size scaling and universality. They are not contained in Eqs. (10) and (14).

Acknowledgments

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