Critical Casimir force in slab geometry with finite aspect ratio: 
Analytic calculation above and below $T_c$

V. DOHM\textsuperscript{(a)}

Institute for Theoretical Physics, RWTH Aachen University - D-52056 Aachen, Germany, EU

received 18 February 2009; accepted in final form 20 March 2009
published online 24 April 2009

PACS 05.70.Jk - Critical point phenomena
PACS 64.60.-i - General studies of phase transitions
PACS 75.40.-s - Critical-point effects, specific heats, short-range order

Abstract – We study the critical Casimir force in a $d$-dimensional $L^2_{∥} \times L$ slab geometry with a finite aspect ratio $\rho = L/L_{∥}$ above, at, and below $T_c$ on the basis of the O($n$) symmetric isotropic $\varphi^4$ field theory with short-range interactions. Exact results are obtained in the large-$n$ limit. For $n = 1$, the result of a perturbation approach at fixed dimension $d = 3$ is presented that describes the dependence on the aspect ratio in the range $\rho \gtrsim 1/4$. Our analytic result for the Casimir force scaling function for $\rho = 1/4$ agrees well with recent Monte Carlo data for the three-dimensional Ising model in slab geometry with periodic boundary conditions above, at, and below $T_c$.

In the presence of fluctuations with long-range correlations, the so-called Casimir forces occur in macroscopic confined systems. The existence of such forces due to long-range critical fluctuations has been predicted by Fisher and de Gennes [1] for fluid films. These forces have attracted theoretical and experimental interest because of their universal features [2,3]. For systems with isotropic short-range interactions, the critical Casimir forces are indeed largely universal as they depend only on the boundary conditions, on the geometry of the confining surfaces and on the universality class of the critical point, except for exponentially small nonuniversal contributions [4].

For fluid films the critical Casimir forces are predicted to be less universal as they are also affected by the nonuniversal van der Waals interactions in the asymptotic critical region away from $T_c$ [4,5]. For anisotropic systems of the same universality class (e.g., magnetic systems with noncubic symmetry), however, two-scale factor universality is absent [4,6–8] and the critical Casimir forces are nonuniversal in the entire critical region as they depend on microscopic couplings even right at $T_c$ [4,6,7,9].

Considerable theoretical effort has been devoted to the study of critical Casimir forces in isotropic film systems with short-range interactions over the past two decades [10–12]. In this paper, we shall focus on the Ising universality class with periodic boundary conditions for which detailed Monte Carlo (MC) data [13,14] are available. While progress has been achieved by means of the $\varepsilon = 4 - d$ expansion [10,12] above the bulk critical temperature $T_c$ no theoretical prediction is available as of yet for the region below $T_c$. The most interesting feature is the existence of a pronounced minimum of the finite-size scaling function of the Casimir force below $T_c$ [13,14], which is characteristic also for the other film systems with realistic boundary conditions [2,3,11,14–16]. In this letter, we present the result of a renormalization-group calculation within the framework of the $\varphi^4$ theory at fixed dimension $d = 3$ [4,17] that is in good agreement with the MC data [13,14], including the minimum below $T_c$ and the Casimir amplitude at $T_c$.

All the existing theoretical studies [10–12] of the critical Casimir force in film systems have considered an $\infty^2 \times L$ geometry. This geometry is, of course, an idealization that is only approximately realized in experiments or in computer simulations. In fact, the MC simulations for the Ising universality class with periodic boundary conditions [13,14] have been carried out for periodic $L^2_{∥} \times L$ slabs with finite aspect ratios $\rho = L/L_{∥}$ in the range $1/4 \leq \rho \leq 1/3$. Most of the available data are for $\rho = 1/6$. This appears to be well justified as the dependence on $\rho$ for $\rho \ll 1$ is expected to be rather weak. In ref. [13] it was stated explicitly that the MC results for $\rho = 1/4$ can hardly be distinguished from those for smaller values of $\rho$.

Our novel approach to the problem takes advantage of the fact that an $L^2_{∥} \times L$ finite-slab geometry is conceptually simpler than a $\infty^2 \times L$ film geometry for two fundamental

\textsuperscript{(a)}E-mail: vdohm@physik.rwth-aachen.de

Copyright © EPLA, 2009
reasons. First, there exists no film transition at finite \( \rho > 0 \), thus there is no necessity of dealing with the difficult problem of dimensional crossover between the three-dimensional bulk transition and the two-dimensional film transition. Second, for \( \rho > 0 \), the system has a discrete mode spectrum with only one single lowest mode, in contrast to the more complicated situation of a lowest-mode \textit{continuum} in film geometry. This opens up the opportunity of building upon the advances that have been achieved in the description of finite-size effects in systems that are finite in all directions [4,18–21]. It is not clear \textit{a priori}, however, in what range of \( \rho \) such a theory is reliable since, ultimately, for sufficiently small \( \rho \ll 1 \), the concept of separating a single lowest mode must break down. Therefore, as a crucial part of our theory, we first provide quantitative evidence for the expected range of applicability of our theory at finite \( \rho \).

We start from the standard \( O(n) \) symmetric isotropic Landau-Ginzburg-Wilson Hamiltonian,

\[
H = \int d^d r \left[ \frac{\rho_0}{2} \nabla \varphi^2 + \frac{1}{2}(\nabla \varphi)^2 + u_0(\varphi^2)^2 \right]
\]

(1)

for the \( n \) component vector field \( \varphi(r) \) in a \( d \)-dimensional \( L_d \times L \) finite-slab geometry with periodic boundary conditions in all directions. The fundamental quantity from which the critical Casimir force can be derived is the singular part \( f_0(t,L,L_0) \) of the free energy \( f \) per unit volume and per component, divided by \( k_B T \). The expected asymptotic (large \( L \), large \( L_0 \), small \( t = (T - T_c)/T_c \)) finite-size scaling form of \( f_0 \) for isotropic systems is [22]

\[
f_0(t,L,L_0) = L^{-d} F(x,\rho)
\]

(2)

with the scaling variable \( x = t(L/\xi_0)^{1/d} \), where \( \xi_0 \) is the amplitude of the second-moment bulk correlation length above \( T_c \).

To study the \( \rho \) dependence of the scaling function \( F(x,\rho) \) we first consider the large-\( n \) limit (at fixed \( u_0 n \)). As an exact result we find in three dimensions

\[
F(x,\rho) = (8\pi)^{-1} \left[ \frac{2}{3} x P^2 \right] + \frac{1}{2} G_0(P^2,\rho),
\]

(3)

\[
G_j(P^2,\rho) = (4\pi^2)^{-1} \int_0^\infty dz z^{j-1} \exp \left( -\frac{P^2 z}{4\pi^2} \right)
\]

\[
\times \left\{ \frac{\rho K(z)}{z} \right\} \right\},
\]

(4)

with \( K(z) = \sum_{m=-\infty}^{\infty} \exp(-zm^2) \), where \( P(x,\rho) \) is determined implicitly by \( P = x - 4\pi G_1(P^2,\rho) \).

The amplitude \( F(0,\rho) \) at \( T_c \) for \( n = \infty \) in three dimensions is shown as thin solid line in fig. 1. This interpolates smoothly between the limits of \( \rho = 0 \) (film) and \( \rho = 1 \) (cube). It is a monotonically decreasing function of \( \rho \), since the value of \( F(0,\rho) \) is suppressed as the confinement becomes stronger. As a nontrivial feature, fig. 1 exhibits a negligible dependence on \( \rho \) for small \( \rho \) up to \( \rho \lesssim 1/4 \). The weak dependence of \( F(x,\rho) \) on \( \rho \) for \( \rho \lesssim 1/4 \) also pertains to the central finite-size region \( |x| \lesssim O(1) \) around \( T_c \). This suggests that studying \( F(x,\rho) \) in a finite-slab geometry with \( \rho = 1/4 \) should yield a good approximation to \( F(x,0) \) in film geometry near bulk \( T_c \).

One expects that a similar situation holds for \( n = 1 \). This is indeed supported by our analytic prediction for \( F(0,\rho) \), as given in eq. (9) below which is shown in fig. 1 as thick solid and dotted lines. We have derived this result on the basis of an improved version [4] of the lowest-mode separation approach [18–21]. Our result for \( F(0,\rho) \) agrees very well with earlier MC data [23] in a cubic geometry at \( \rho = 1 \) (full circle in fig. 1). In the range \( \rho > \rho_{\text{max}} = 0.247 \) (thick solid line), \( F(0,\rho) \) has the expected negative slope. In the range \( \rho < \rho_{\text{max}} = 0.247 \), however, the positive slope of the dotted portion of the curve constitutes a clear indication for the expected deterioration of the quality of the lowest-mode separation approach. Thus, we consider the existence of a maximum of the \( n = 1 \) line at a finite value of \( \rho = \rho_{\text{max}} = 0.247 \) as an artifact of the lowest-mode separation approach. In a flat geometry with \( L/L_0 \ll 1/4 \), the system is already close to film geometry such that the higher modes are not well separated from the single lowest mode. On the other hand, together with the result for \( n = \infty \), fig. 1 suggests that a calculation of \( F(x,\rho) \) for \( n = 1 \) at \( \rho = 1/4 \) should yield an acceptable approximation to \( F(x,0) \) in film geometry near bulk \( T_c \).

Our derivation of \( F(x,\rho) \) for \( n = 1 \) is based on the Hamiltonian (1) where the decomposition \( \varphi = \Phi + \sigma \) is made into a homogeneous lowest-mode amplitude \( \Phi \) and higher-mode fluctuations \( \sigma \). After integration over \( \sigma \), the free energy density is obtained in the form

\[
f = f_0 - V^{-1} \ln \int_{-\infty}^{\infty} d\Phi \exp [-H_0(\Phi) - \Gamma(\Phi)],
\]

(5)
with \( H_0(\Phi) = V \left( \frac{1}{2} r_0 \Phi^2 + u_0 \Phi^4 \right) \), where \( f_0 \) is independent of \( r_0 \) and \( u_0 \). The higher-mode contribution \( \Gamma(\Phi) \) is calculated in one-loop order and expanded around the lowest-mode average \( M_0^2 = \int d\Phi \Phi^2 e^{-H_0}/\int d\Phi e^{-H_0} \) up to \( O((\Phi^2 - M_0^2)^2) \). In truncating our expansion of \( \Gamma(\Phi) \) we require that, in the central finite-size region including \( T = T_c \), the terms of \( O(u_0^2) \) are neglected. As we are working at fixed dimension \( 2 < d < 4 \) there is no necessity of further expanding the exponential function \( e^{-H_0 - T} \). Thus, we maintain the exponential structure of the integrand in (5). The resulting bare perturbation expression for \( f \) contains the bare bulk free energy density \( f_b^\pm \equiv \lim_{T \to \infty} f \) in one-loop order above (+) and below (−) \( T_c \). The dependence of \( f_b^\pm \) on the aspect ratio \( \rho \) appears i) on the level of the lowest-mode Hamiltonian \( H_0(\Phi) \) and ii) on the level of the contribution of \( \Gamma(\Phi) \). The former dependence i) comes from \( \int d\rho |L(\rho)|^{-1/2} |\vartheta(y)| \) with \( y_0 = y_0(L(\rho)^{-1/2}/u_0)^{1/2} \), where

\[
\vartheta(y) = \int_0^\infty dz z^2 e^{-y z^2} \int_0^\infty dz e^{-y z^2} z^4. \tag{6}
\]

The latter dependence ii) is contained in the difference between sums over higher modes and bulk integrals in wave vector (\( k \)) space such as

\[
V^{-1} \sum_{k > 0} (r_0 + k^2)^{-m} - \frac{1}{2} \int d^4 k \left( \frac{2\pi^2}{m} \right)^2 (r_0 + k^2)^{-m} = m^{2m-2} \rho^2 \nu \left( \frac{2\pi^2}{m} \right)^2 m (r_0 L^2, \rho), \tag{7}
\]

\[
I_m(r_0 L^2, \rho) = f_0^\pm dz z^m \exp \left[ -r_0 L^2 z^2 / 4(2\pi)^2 \right] \times \left\{ \rho K(\rho^2 z) \right\} \left[ K(\rho^2 z) - (\rho/z)^{d/2} - 1 \right]. \tag{8}
\]

The bare perturbation result needs, of course, to be renormalized. Within the minimal renormalization scheme in three dimensions [17] we have obtained the following scaling function for \( n = 1 \):

\[
F(x, \rho) = -\frac{t^3}{48\pi} - \frac{\nu Q^2 x^2 \omega^{-\alpha/\nu}}{16\pi \alpha} + \frac{1}{2} G_0(l^2, \rho) + 18 u^* \rho \left| \vartheta(y) \right|^2 + (\rho^2 - 1) \left\{ a(x, \rho) + a(x, \rho) \right\}^2 - b(x, \rho) I_1(l^2, \rho) - b(x, \rho)^2 I_2(l^2, \rho) - \rho^2 \ln \int_{-\infty}^{\infty} dz \exp \left[ -\frac{1}{2} Y(x, \rho) z^2 - z^4 \right] \frac{\rho^2}{2} \left\{ \frac{l^2}{m} \left| 1 + 18 u^* R_2(l, \rho) \right| \right\}, \tag{9}
\]

where

\[
Y(x, \rho) = \frac{l^3}{2} \rho^{-1} (4\pi u^*)^{-1} \left\{ 24 u^* a(x, \rho) R_2(l, \rho) + Q^* x l^{-1/\nu} \left\{ 1 + 18 u^* R_2(l, \rho) \right\} + 12 u^* R_1(l, \rho) \right\}, \tag{10}
\]

with \( a(x, \rho) = 12u^{1/2} l^{-3/2} \rho^{1/2} \vartheta(y) \) and \( b(x, \rho) = 3l^{1/2} u^{1/2} \rho^{-1/2} \vartheta(y) \), \( u^* = 0.0412, \) \( Q^* = 0.945, \) and \( \nu = (2 - \alpha)/3 = 0.6335 \).

The functions \( t(x, \rho), y(x, \rho), \) and \( R_l(l, \rho) \) are determined by

\[
y = x Q^* l^{-\alpha/\nu} |\vartheta(y)|^{-1/2}, \tag{11}
\]

\[
y = x Q^* l^{-\alpha/\nu} |\vartheta(y)|^{-1/2}, \tag{12}
\]

\[
R_l(l, \rho) = 4\pi (1 - \rho^2) l^{-3} + (4\alpha)^{-1} I_l(t, \rho), \tag{13}
\]

\[
R_2(l, \rho) = -\frac{1}{2} + 4\pi (1 - \rho^2) l^{-3} + (4\alpha)^{-1} I_2(t, \rho). \tag{14}
\]

For finite \( \rho > 0 \), \( F(x, \rho) \) is an analytic function of \( x \) near \( x = 0 \), in agreement with general analyticity requirements.

The singular part of the bulk free energy density \( f_b^\pm(t) = A^+ |t|^{d\alpha} \) is, of course, independent of \( \rho \). It can be written as \( f_b^\pm = L^{-d} F_b^\pm(x) \), where \( F_b^\pm(x) \) is the bulk part of \( F(x, \rho) \) which is obtained from (9) in the limit of large \( |x| \). It is given by [4]

\[
F_b^\pm(x) = \left\{ Q_1 |x|^{d
\nu}, \quad \text{for } T > T_c, \right. \tag{15}
\]

\[
\left. \left( A^- / A^+ \right) Q_1 |x|^{d\nu}, \quad \text{for } T < T_c. \right. \tag{15}
\]

with universal numbers \( Q_1 = -0.1197 \) and \( A^- / A^+ = 2.034 \) in three dimensions. Thus, the singular part of the excess free energy density \( f_b^\mp = f_b - f_b^\pm \) has the scaling form

\[
f_b^\pm(t, L, L_\parallel) = L^{-d} F_b^\pm(x, \rho), \tag{16}
\]

\[
F_b^\pm(x, \rho) = F(x, \rho) - F_b^\pm(x). \tag{17}
\]

The prediction of the \( \rho \) dependence of \( F_b^\pm(x, \rho) \) above, at, and below \( T_c \) for the Ising universality class as described by (9)–(17) without any adjustment of parameters is the central result of this paper. This function contains a \( \rho \)-dependent minimum slightly below \( T_c \). The scaling function \( F_b^\pm(x, \rho) \) is shown in fig. 2 for several values of \( \rho \). As expected on the basis of fig. 1, the difference between \( F_b^\pm(x, \rho) \) for \( \rho = 1/3 \) and \( \rho = 1/4 \) is rather small.

By definition, the function \( F_b^\pm(x, \rho) \) has a weak non-analyticity at \( x = 0 \) because of the subtraction of the non-analytic bulk scaling function \( F_b^\pm(x, \rho) \), eq. (15). Note that our analytic result (9) is not expected to be quantitatively reliable for \( \rho < \rho_{\text{max}} = 0.247 \) for the reasons mentioned above in the context of fig. 1. Furthermore, the universal scaling structures (2) and (16) are not valid in the large-\( |x| \) regimes where the excess free energy density \( f_b^\pm \) has an exponential dependence \( \propto \exp(-|\xi_{b\parallel}| / L) \) on the nonuniversal bulk correlation lengths \( \xi_{b\parallel} \) above and below \( T_c \) [4]. The same reservations should be made for the scaling structure of the critical Casimir force to be presented in (18) below.

We note that so far no confirmation of the theory at \( \rho = 1 \) [4] by MC simulations has been presented except right at \( T = T_c \) [23]. In particular, the prediction of a minimum of \( F(x, 1) \) below \( T_c \) for \( \rho = 1 \) [4] is as yet unconfirmed since no MC data are available as of yet in

20001-p3
this regime. For this reason, it is particularly interesting to present here our prediction of a minimum of the Casimir force scaling function for small ρ slightly below Tc, which can be compared with the recent MC data [13,14].

We define the critical Casimir force $F_{\text{Casimir}}$ per unit area in a finite-slab geometry as

$$F_{\text{Casimir}}(t, L, Lt) = -\frac{\partial [L F_{\text{ex}}]}{\partial L} = L^{-d} X(x, \rho),$$

(18)

where the derivative is taken at fixed $L_{\parallel}$. This definition is equivalent to its lattice counterpart introduced in [14]. The Casimir force scaling function $X$ can then be expressed in terms of $F_{\text{ex}}$ as

$$X(x, \rho) = (d - 1) F_{\text{ex}}(x, \rho) - \frac{x}{\nu} \frac{\partial F_{\text{ex}}(x, \rho)}{\partial x} - \rho \frac{\partial F_{\text{ex}}(x, \rho)}{\partial \rho}.$$  

(19)

Numerical evaluation of (19) yields the curve shown in fig. 3. There is good overall agreement with the MC data of [14] (with $\rho = 1/6$ and $L = 20$) and with the MC data of [13] (not shown in fig. 3) in the range $-2 \leq x \leq 16$. Somewhat unexpectedly, our result exhibits a small shoulder near $T_c$. This shoulder is not present in the scaling function of the excess free energy density $F_{\text{ex}}(x, \rho)$ (fig. 2) but arises through the derivative term $-(x/\nu) \partial F_{\text{ex}}(x, \rho)/\partial x$. This small shoulder of our function $X(x, \rho)$ turns into a small local maximum for $\rho > 1/4$ at $x = 0$. It remains to be seen whether this feature is confirmed by MC simulations for $\rho > 1/4$. As already expected on the basis of the line of reasoning given in the context of fig. 1, the agreement of our function $X(x, \rho)$ with the MC data of [14] shown in fig. 3 indeed deteriorates if $\rho$ is taken to be smaller than $\rho_{\text{max}} = 0.247$.

A more detailed comparison with earlier results is shown in fig. 4. Most significant is the excellent agreement of the position of the minimum of our theoretical curve $x_{\text{min}} = -0.608$ with the MC estimate [14] $x_{\text{min}}^{\text{MC}} = -0.681$ (full circle in fig. 4). There is also reasonable agreement with regard to the depth of the theoretical minimum $X(x_{\text{min}}, 1/4) = -0.345$ compared to the MC estimate [14] $X_{\text{min}}^{\text{MC}} = -0.329$ (full circle in fig. 4). Furthermore, our result $X(0, 1/4) = -0.326$ at $T_c$ is in substantially improved agreement with the MC estimate [14] $X_{\text{MC}}^{T_c} = -0.304$ at $T_c$ (triangle in fig. 4), compared to the earlier $\epsilon$ expansion results $-0.221$ in two-loop order [10] and $-0.393$ in three-loop order [12] for film geometry $\rho = 0$ (shown in fig. 4 as dashed and dotted lines, respectively).

In summary, we have presented a novel approach to the analytic calculation of the critical Casimir force scaling function in slab geometry for isotropic systems with short-range interactions in the Ising universality class and have obtained quantitative agreement with MC data for periodic boundary conditions. This approach can be
extended to realistic boundary conditions and to other universality classes which may then lead to a satisfactory explanation of the minimum of the critical Casimir force scaling function below $T_c$ in real systems [15].

***

The author is grateful to S. Dietrich and A. Gambassi for providing the MC data of ref. [14] in numerical form.

REFERENCES

[1] Fisher M. E. and de Gennes P. G., C. R. Seances Acad. Sci. Ser. B, 287 (1978) 207.
[2] Hertlein C., Helden L., Gambassi A., Dietrich S. and Bechinger C., Nature (London), 451 (2008) 172.
[3] For reviews see Krech M., The Casimir Effect in Critical Systems (World Scientific, Singapore) 1994; J. Phys.: Condens. Matter, 11 (1999) R391; Gambassi A., arXiv:0812.0935 [cond-mat.stat-mech] (2008).
[4] Dohm V., Phys. Rev. E, 77 (2008) 061128.
[5] Chen X. S. and Dohm V., Phys. Rev. E, 66 (2002) 016102; Physica B, 329-333 (2003) 202; Dantchev D., Krech M. and Dietrich S., Phys. Rev. E, 67 (2003) 066120; Dantchev D., Diehl H. W. and Gr"uneberg D., Phys. Rev. E, 73 (2006) 016131; Dantchev D., Schlesener F. and Dietrich S., Phys. Rev. E, 76 (2007) 011121.
[6] Chen X. S. and Dohm V., Phys. Rev. E, 70 (2004) 056136.
[7] Dohm V., J. Phys. A, 39 (2006) L259.
[8] Selke W. and Schichur L. N., J. Phys. A, 38 (2005) L739.
[9] Dantchev D. and Gr"uneberg D., Phys. Rev. E, 79 (2009) 041103.
[10] Krech M. and Dietrich S., Phys. Rev. Lett., 66 (1991) 345; Phys. Rev. A, 46 (1992) 1886; 192.
[11] Borjan Z. and Upton P. J., Phys. Rev. Lett., 81 (1998) 4911; 101 (2008) 125702; Zandi R., Rudnick J. and Kardar M., Phys. Rev. Lett., 93 (2004) 155302; Zandi R., Shackell A., Rudnick J., Kardar M. and Chayes L. P., Phys. Rev. E, 76 (2007) 036001(R); Schmidt F. M. and Diehl H. W., Phys. Rev. Lett., 101 (2008) 100601.
[12] Diehl H. W., Gr"uneberg D. and Shipot M. A., Europhys. Lett., 75 (2006) 241; Gr"uneberg D. and Diehl H. W., Phys. Rev. B, 77 (2008) 115409.
[13] Dantchev D. and Krech M., Phys. Rev. E, 69 (2004) 046119.
[14] Vasilyev O., Gambassi A., Maciolek A. and Dietrich S., EPL, 80 (2007) 60009; arXiv:0812.0750 [cond-mat.stat-mech] (2008).
[15] Garcia R. and Chan M. H. W., Phys. Rev. Lett., 83 (1999) 1187; Ganshin A., Scheidemantel S., Garcia R. and Chan M. H. W., Phys. Rev. Lett., 97 (2006) 075301; Fukuto M., Yano Y. F. and Pershan P. S., Phys. Rev. Lett., 94 (2005) 135702.
[16] Hutch A., Phys. Rev. Lett., 99 (2007) 185301.
[17] Dohm V., Z. Phys. B, 60 (1985) 61; 61 (1985) 193; Schloms R. and Dohm V., Nucl. Phys. B, 328 (1989) 639; Phys. Rev. B, 42 (1990) 642.
[18] Brežin E. and Zinn-Justin J., Nucl. Phys. B, 25 (1985) 867.
[19] Rudnick J., Guo H. and Jasnow D., J. Stat. Phys., 41 (1985) 353.
[20] Esser A., Dohm V., Hermes M. and Wang J. S., Z. Phys. B, 97 (1995) 205.
[21] Esser A., Dohm V. and Chen X. S., Physica A, 222 (1995) 355.
[22] Privman V. and Fisher M. E., Phys. Rev. B, 30 (1984) 322.
[23] Mon K. K., Phys. Rev. Lett., 54 (1985) 2671; Phys. Rev. B, 39 (1989) 467.