Order-Parameter Profiles and Casimir Amplitudes in Critical Slabs

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A critical phase confined between two parallel plates, with symmetry-breaking fields h_1 and h_2 acting on each plate, is considered for (i) $h_1 h_2 > 0$ (denoted $ab = ++$) and (ii) $h_1 h_2 < 0$ ($ab = +-$). Using local-functional methods, we calculate order-parameter scaling functions $\Psi_{ab}(x)$ and Casimir amplitudes A_{ab}, for *general* dimension d. At $d = 2$, our $\Psi_{++}(x)$ almost coincides with *exact* conformal predictions. For the Ising universality class, we obtain expansions for A_{ab} in $\epsilon = 4 - d \downarrow 0$ in excellent agreement with those obtained from field theory and, in $d = 3$, new results are presented for A_{ab} and $\Psi_{ab}(x)$. [S0031-9007(98)07753-9]

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The Casimir effect, occurring when either a quantum field or a thermodynamic system at its bulk critical point is confined between two plates, has generated a great deal of interest in both quantum field theory and statistical physics [1]. Consider a statistical system, at its bulk critical point at temperature T_c, consisting of a slab contained between two parallel plates of area A and separated by distance L. Let $z \in [0, L]$ denote the perpendicular distance of a point inside the slab from one of the plates. If F is the free energy of the system, the *reduced incremental free energy*, $f^\times$, is defined as

$$f^\times(L) := \lim_{A\to\infty} \frac{F}{k_B T_c A} - L f_b \,, \qquad (1)$$

where f_b is the reduced *bulk* free-energy density. Fisher and de Gennes [2] predicted that $f^\times(L)$ takes the form

$$f^\times(L) \approx \Sigma_1 + \Sigma_2 + A_{ab} L^{1-d^*} + \dots \qquad (2)$$

as $L \to \infty$ where $d^* := (2 - \alpha)/\nu$ with α and ν being the usual specific heat and correlation length critical exponents and Σ_1 and Σ_2 are critical *wall tensions* coming from the two plates. Throughout, the subscript a (respectively, b) refers to the boundary condition on the plate at $z = 0$ (respectively, $z = L$). Assuming hyperscaling, $d^* = d$ (i.e., the spatial dimension) for $2 \le d \le d_>$ and $d^* = d_>$ for all $d \ge d_>$ where $d_>$ is the upper critical dimension of the system. For the Ising universality class, $d_> = 4$. It was later argued that the *Casimir amplitude*, A_{ab}, is a universal number for $d < d_>$ [3] (see also [4]), and a great deal of effort has gone into calculating this amplitude for various universality classes (see [1] and references therein). Suggested experimental approaches in, e.g., critical fluids include measuring A_{ab} *directly* using atomic force microscopes or *indirectly* from wetting experiments (see [1]).

In this Letter, we shall consider only those slabs where an external symmetry-breaking boundary field has been applied to *both* plates—i.e., a field h_1 (respectively, h_2) acting on the plate at $z = 0$ (respectively, $z = L$). It has been noted (see Ref. [1]) that if a symmetry-breaking boundary condition acts on at least one of the plates then a field-theoretic expansion in $\epsilon = 4 - d$ applied to the $O(N)$ symmetric ϕ^4 theory (this, of course, includes Ising uniaxial ferromagnets) shows that $A_{ab} \approx \bar{A}_{ab}\epsilon^{-1}$ as $\epsilon \downarrow 0$. This corresponds to a logarithmic anomaly in the large L behavior of $f^\times(L)$ when $d = d_> = 4$, in which case the term $A_{ab}L^{1-d^*}$ in Eq. (2) is replaced by $\bar{A}_{ab}L^{-3}\ln L$.

One can also define critical order-parameter profile scaling functions as follows. If $m(z; L)$ is the order-parameter density as a function of z at the bulk critical point (e.g., the magnetization of a magnet) then as $z \to \infty$ and $L \to \infty$, keeping $0 < z/L < 1$, we have for a given boundary condition ab

$$m(z; L) \approx M_{ab} L^{-\beta/\nu} \Psi_{ab}(z/L) \,, \qquad (3)$$

where β is the usual spontaneous magnetization exponent and the scaling function, $\Psi_{ab}(x)$, is *universal* once its normalization has been selected by specifying the *nonuniversal* amplitude M_{ab}. Conformal invariance has yielded exact predictions on the form of $\Psi_{ab}(x)$ in $d = 2$ for various boundary conditions [5–7] and also, for general $d < d_>$, it has been seen that the short distance behavior of $\Psi_{ab}(x)$ can be simply related to A_{ab} via the short-distance expansion [8,9].

Here we shall always set $h_1 > 0$ and consider just two types of boundary condition on the other plate: (i) $h_2 > 0$ denoted by $ab = ++$ and (ii) $h_2 < 0$ denoted by $ab = +-$. The nonuniversal amplitudes, M_{ab}, are chosen so that $\Psi_{++}(1/2) = 1$ and the derivative $\Psi'_{+-}(1/2) = -1$ [by antisymmetry, $\Psi_{+-}(1/2) = 0$]. The Casimir amplitudes and profile scaling functions are then determined using a relatively newly developed method [10] based on local free-energy functionals of the order-parameter density, $m(z)$, suitably adapted to cope with *nonclassical* criticality (i.e., for $d \le d_>$). The method is *nonperturbative* and can be applied directly to $d = 3$—an advantage over field-theoretical ϵ expansions which require extrapolating to $d = 3$—thus yielding new reliable results at the physically interesting dimension as well as at $d = 2$. But it can also be used to generate expansions in ϵ for $d \uparrow d_>$. Hence, we can significantly substantiate our

$d = 3$ predictions by making detailed comparisons with the results of conformal invariance [5–7,11,12] at $d = 2$ and with the recently derived field-theoretical ϵ expansions for A_{++} and A_{+-} [13].

Following Ref. [10] we start by asserting that the magnetization profile, $m(z)$, minimizes a free-energy functional, $\mathcal{F}[m]$, of the following form:

$$\mathcal{F}[m] = \int_0^L \mathcal{A}(m, \dot{m})\, dz + f_1(m_1) + f_2(m_2), \quad (4)$$

where $\dot{m} := dm/dz$, $m_1 := m(0)$, $m_2 := m(L)$, $f_j(m_j)$ for $j = 1, 2$, coming from the respective walls, has the form $f_j(m_j) = -h_j m_j + \ldots$ and $f^{\times}(L) = \min_{[m]} \mathcal{F}[m]$. Mean-field theory is obtained by choosing $\mathcal{A}(m, \dot{m})$ of squared-gradient Landau type. In order to go beyond mean-field theory for dimensions $d \le d_{>}$ Fisher and Upton [10] considered integrands of the form

$$\mathcal{A}(m, \dot{m}) = \{1 + J(m)\mathcal{G}[\dot{m}\Lambda(m)]\}W(m), \quad (5)$$

where $W(m) := \Phi(m) - \Phi(m_{\rm b})$ with $\Phi(m)$ being the Helmholtz free energy density and $m_{\rm b}$ the bulk magnetization. By symmetry, $\mathcal{G}(x)$ must be an even function of x with $\mathcal{G}(0) = 0$. Since scale invariance plays such an important role at bulk critical points one insists that the dimensionless combinations $J(m)$ and $\dot{m}\Lambda(m)$ be scale-free. Several possible choices for $J(m)$ and $\Lambda(m)$ have been considered [10], the simplest being $J(m) = 1$ and $\Lambda(m) = \xi(m)/\sqrt{2\chi(m)W(m)}$ where $\xi(m)$ and $\chi(m)$ are, respectively, the bulk correlation length and susceptibility for a homogeneous system with magnetization m. From a field theoretical point of view, the integral $\int \mathcal{A}(m, \dot{m})\, dz$ in (4) can be regarded as a *local* approximation to the vertex generating functional (or effective action) $\Gamma[\varphi = m(z)]$ with the integrand (5) heuristically constructed, though made to satisfy numerous desiderata [10].

Although much is known about the bulk quantities $W(m)$, $\chi(m)$, and $\xi(m)$, which enter the local functional, one now needs to know something of the form $\mathcal{G}(x)$ takes. This was not the case in previous applications of this method [10,14] to semi-infinite geometries where details of $\mathcal{G}(x)$ were unimportant. It has been established, however, that $\mathcal{G}(x)$ must satisfy several conditions [10]. These include the following expansion:

$$\mathcal{G}(x) = x^2 + \sum_{j=2}^{\infty} G_{0,j} x^{2j} \quad \text{as } x \to 0, \quad (6)$$

which follows from standard considerations based on gradient expansions in density functional theory [15]. Also, in order that $m(z)$ remains analytic in z as m passes through zero, such as occurs in the $ab = +-$ boundary condition, we must have [10]

$$\mathcal{G}(x) + 1 = G_\infty x^{2-\tilde{\eta}} \left(1 + \sum_{j=1}^{\infty} G_{\infty,j} x^{-j\tau} \right) \quad (7)$$

as $x \to \infty$ where $\tilde{\eta} = 2\eta/(d^* + \eta)$ and $\tau = 2\beta/(\beta + \nu)$ with η being the usual critical correlation function exponent. Finally, in semi-infinite geometry, in order that critical adsorption profiles have the correct exponential decay for temperatures away from $T_{\rm c}$ and that thermodynamic consistency holds off coexistence, it is required that [10]

$$\mathcal{G}(1) = 1, \qquad \mathcal{G}'(1) = 2. \quad (8)$$

It is possible to write down expressions for $\mathcal{G}(x)$ which *fully* satisfy all three requirements (6)–(8) [16] but the following *approximant* was found to be adequate for our purposes:

$$(2 - \tilde{\eta})\mathcal{G}(x)/2 = [1 + x^2 R_{[n/n]}(x^2)]^{(2-\tilde{\eta})/2} - 1, \quad (9)$$

where $R_{[n/n]}(x^2) = P_n(x^2)/Q_n(x^2)$ with $P_n(\cdot)$ and $Q_n(\cdot)$ being polynomials of degree n (usually one needs $n \ge 2$) having $P_n(0) = Q_n(0) = 1$. Clearly, (9) completely satisfies (6), and it captures the leading term on the right-hand side of (7). Condition (8) can be imposed by adjusting the polynomial coefficients in $R_{[n/n]}(\cdot)$. One requires that simple squared-gradient theory, $\mathcal{G}(x) = x^2$, follows when $\eta = \tilde{\eta} = 0$. Typical plots of $\mathcal{G}(x)$, for the Ising universality class (see [17]), based on this approximant are shown in Fig. 1. One notices that $\mathcal{G}(x)$ is virtually indistinguishable from x^2 when $0 \le x \le 1$ even when enlarging the graph at this range of x to a much bigger size.

We now present the solution of the variational problem needed to extremize $\mathcal{F}[m]$. The first thing to note is that the Euler-Lagrange equations for functionals of the type in (4) [where there is no explicit z dependence in $\mathcal{A}(m, \dot{m})$] have a first integral given by the following ordinary differential equation determining the profile $m(z)$

$$\dot{m}\,\frac{\partial \mathcal{A}}{\partial \dot{m}} - \mathcal{A} = E(L), \quad (10)$$

which expresses an "energy" conservation law in the mechanical analog with the constant $E(L)$ [with

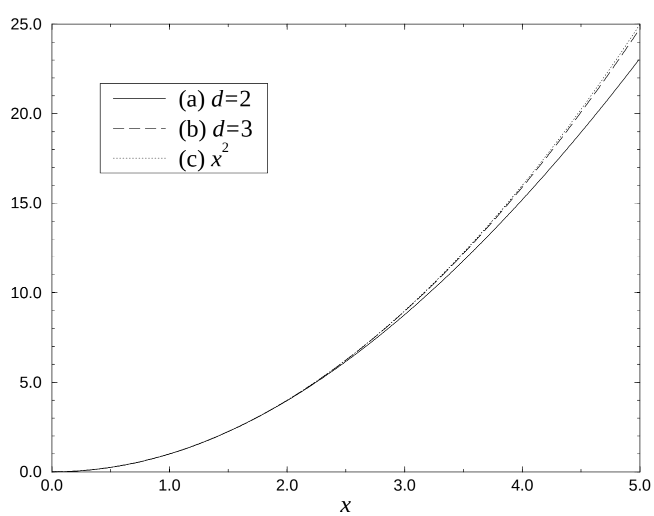

FIG. 1. Plots of $\mathcal{G}(x)$ based on approximant (9) with $n = 2$ for (a) $d = 2$ and (b) $d = 3$. Here, the polynomials $P_2(y) = 1 + p_1 y + p_2 y^2$ and $Q_2(y) = 1 + q_2 y^2$ were used and (p_1, p_2, q_2) determined by imposing (8) and fixing $G_\infty = 1$. The curve x^2 is plotted as (c) for comparison.

$\lim_{L\to\infty} E(L) = 0]$ corresponding to the energy. From the boundary (and other) conditions, $E(L)$ can be determined and hence the profiles $m(z;L)$. When determining $f^{\times}(L)$, and therefore the Casimir amplitudes, the calculations are greatly simplified by noting the relation [18]

$$\frac{\partial f^{\times}}{\partial L} + E(L) = 0\,, \tag{11}$$

which corresponds to a Hamilton-Jacobi-like equation in the mechanical analog which, we stress, is true for quite general $\mathcal{A}(m,\dot{m})$ provided it has no explicit z dependence. Thus, when taking scaling limits, $z \to \infty$, $L \to \infty$, at the bulk critical point, $E(L)$ for large L plays a pivotal role in determining both $\Psi_{ab}(x)$ and A_{ab}.

The results will be expressed in terms of the function $\hat{\mathcal{G}}(x)$, defined as $\hat{\mathcal{G}}(x) := x\mathcal{G}'(x) - \mathcal{G}(x)$, and its inverse $\hat{\mathcal{G}}^{-1}(x)$, i.e., $\hat{\mathcal{G}}[\hat{\mathcal{G}}^{-1}(x)] = x$. Also, we define the functions $J_{++}(y)$ and $J_{+-}(y)$ by

$$J_{+\pm}(y) := \int_y^{\infty} \frac{|u|^{-(1+\nu/\beta)}\,du}{|\hat{\mathcal{G}}^{-1}(1 \mp |u|^{-d^*\nu/\beta})|}\,, \tag{12}$$

where $y \geq 1$ for $++$ and $y \in (-\infty,\infty)$ for $+-$. Applying the scaling limit to (10) at the critical point determines the scaling functions, $\Psi_{+\pm}(x)$, which can be expressed as

$$\Psi_{++}(x) = J_{++}^{-1}[2J_{++}(1)x]\,, \tag{13a}$$

$$\Psi_{+-}(x) = c_1 J_{+-}^{-1}[2J_{+-}(0)x]\,, \tag{13b}$$

where $J_{+\pm}^{-1}(\cdot)$ are the inverse functions and the constant c_1 is given by

$$c_1 = [(1-\tilde{\eta})G_{\infty}]^{1/(2-\tilde{\eta})}/2J_{+-}(0)\,. \tag{14}$$

Note that, given $\mathcal{G}(\cdot)$, $\Psi_{+\pm}(x)$ depend *solely* on β/ν and d^*. Similarly, taking the large L limit and using (11), we obtain the Casimir amplitudes

$$A_{+\pm} = \frac{\mp R_\xi^c[2\delta(\delta+1)]^{d^*/2}}{(d^*-1)(\delta+1)} \times \begin{cases}[J_{++}(1)]^{d^*},\\ [J_{+-}(0)]^{d^*},\end{cases} \tag{15}$$

where, if along the critical isotherm in the bulk ($T = T_c$, $h \neq 0$) we have, as the bulk field $h \to 0$, the usual relations $h \approx D|m|^{\delta-1}m$ and $\xi \approx \xi_c|h|^{-\nu/\beta\delta}$—thus defining the exponent δ and the critical amplitudes D and ξ_c—then the *bulk* universal amplitude relation, R_ξ^c, is defined as $R_\xi^c := \xi_c^{d^*}D^{-1/\delta}$. The quantity R_ξ^c arrives from hyperscaling and is therefore only universal for $d \leq d_>$. It can be expressed in terms of the more standard bulk amplitude relations [19,20] for which, in the Ising universality class, there exist estimates in $d = 2$ [19] and $d = 3$ [20] and also expansions in $\epsilon = 4 - d$ [19].

Observe, from (12), for the $++$ case that $\hat{\mathcal{G}}^{-1}(x)$, and therefore $\mathcal{G}(x)$ [by its monotone property together with (8)], is only ever evaluated for $0 \leq x \leq 1$, whereas for the $+-$ case $\mathcal{G}(x)$ is required only for $x \geq 1$. Now recall that for all $x \in [0,1]$, $\mathcal{G}(x) \simeq x^2$ to a very good approximation. Thus, putting $\hat{\mathcal{G}}^{-1}(x) = \sqrt{x}$ into (12) for $J_{++}(y)$ gives via (13a)

$$\Psi_{++}(x) = [\psi_{d^*}(x)]^{-\beta/\nu}. \tag{16}$$

Although, of course, β/ν (the bulk scaling dimension) depends on the bulk universality class of the particular system under study, the function $\psi_{d^*}(x)$ is universal in a more general sense in that it depends only on d^* *regardless* of the values of the bulk exponents—a property known to hold for $d = 2$ as a result of conformal invariance [5]. Below, we give expressions for $\psi_{d^*}(x)$ for $d^* = 2, 3, 4$,

$$\psi_2(x) = \sin \pi x\,, \tag{17a}$$

$$\psi_3(x) = \frac{(\sqrt{3}+1)\,\mathrm{cn}[K_3(1-2x);k_3] - \sqrt{3} + 1}{\mathrm{cn}[K_3(1-2x);k_3] + 1}\,, \tag{17b}$$

$$\psi_4(x) = \frac{\mathrm{sn}(2K_4x;k_4)}{\sqrt{2}\,\mathrm{dn}(2K_4x;k_4)}\,, \tag{17c}$$

where $\mathrm{sn}(\cdot;k)$, $\mathrm{dn}(\cdot;k)$, and $\mathrm{cn}(\cdot;k)$ are the standard Jacobian elliptic functions with modulus k, $k_3 = (\sqrt{3}+1)/2\sqrt{2}$, $k_4 = 1/\sqrt{2}$,

$$K_3 = \mathrm{cn}^{-1}\left(\frac{\sqrt{3}-1}{\sqrt{3}+1};k_3\right) \simeq 1.845\,375\ldots\,, \tag{18}$$

and $K_4 = \mathbf{K}(k_4) \simeq 1.854\,07$ where $\mathbf{K}(\cdot)$ is the complete elliptic integral of the first kind. Strikingly, (17a) substituted into (16) gives the *exact* expression for $\Psi_{++}(x)$ as obtained by conformal invariance at $d = 2$ [5]. This is remarkable as one might have expected these local-functional methods to get less reliable the further one reduces d away from the mean-field dimension $d_>$. It is therefore not unfeasible to suppose that (17b) substituted into (16) yields the exact $d = 3$ result for a given β/ν or, if not exact, then it should give, for the first time, an accurate prediction for $\Psi_{++}(x)$ for general (not just Ising) $d = 3$ critical slabs. For the Ising model, (17c) substituted into (16) gives the mean-field result obtained by Krech [13] from Landau theory.

In what now follows, we shall restrict ourselves to the Ising universality class [17]. Results for $\Psi_{+\pm}(x)$, obtained by numerically integrating (12) and (13) and using (9) for $\mathcal{G}(x)$, are plotted in Fig. 2 for $d = 2$, $d = 3$, and $d \geq 4$. Since $\Psi_{++}(x)$ [$\Psi_{+-}(x)$] is (anti)symmetric about $x = 1/2$, results are presented only for the range $0 \leq x \leq 1/2$. For the $++$ case, the curves plotted here are indistinguishable from those obtained using $\mathcal{G}(x) = x^2$, leading to near exact agreement with the conformal results at $d = 2$. However, our $\Psi_{+-}(x)$ at $d = 2$ no longer agrees quite so well with the exact conformal result [6,7]. This reflects the greater uncertainty in the form of $\mathcal{G}(x)$ for $x \gg 1$ which enters in calculations involving the $+-$ case only. In particular, it is uncertain what value G_∞ should take although we found that $G_\infty = 1$ seems to work best. In any case, we expect greater accuracy in $d = 3$.

As for the Casimir amplitudes, Eqs. (15) for $d = 2$ give $A_{++} \simeq -0.0666_7$ and $A_{+-} \simeq 1.586$, and these should be compared with the exact conformal results [11,12] which are $A_{++} = -\pi/48 \simeq -0.065\,45$ and $A_{+-} = 23\pi/48 \simeq 1.505$. Again, agreement is less good

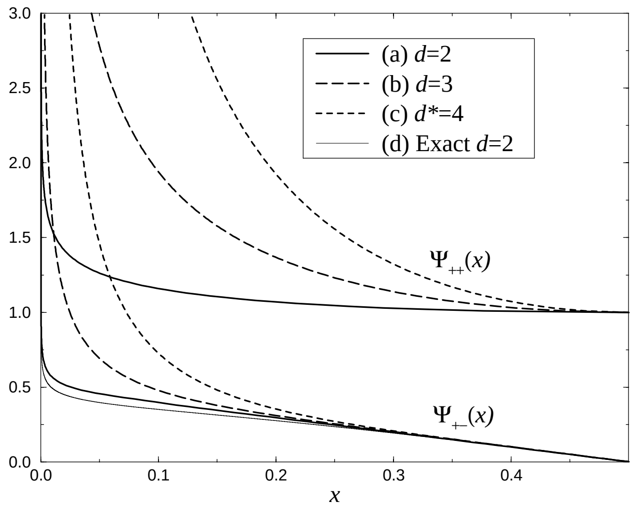

FIG. 2. Plots of $\Psi_{++}(x)$ and $\Psi_{+-}(x)$ for the Ising universality class at (a) $d = 2$, (b) $d = 3$, and (c) $d \geq 4$ (mean-field theory). For comparison, plotted as (d) are the exact $d = 2$ profiles, $\Psi_{++}(x) = (\sin \pi x)^{-1/8}$ [which coincides exactly with (a)] and $\Psi_{+-}(x) = \pi^{-1}(\sin \pi x)^{-1/8} \cos \pi x$, both obtained by conformal invariance.

for the $+-$ case and the (small) error in the $++$ case may well reflect deficiencies in estimates for the bulk quantity R_ξ^c. For $d = 3$, we obtain $A_{++} \simeq -0.42_8$ and $A_{+-} \simeq 3.1$ which should be compared with the Monte Carlo results of Krech [13] who quotes $A_{++} \simeq -0.35$ and $A_{+-} \simeq 2.45$ but one should be wary of large finite-size corrections in the Monte Carlo data. One can also use Eqs. (15) to generate expansions in $\epsilon = 4 - d$ and thus obtain

$$A_{++} = \frac{-3K_4^4}{2\pi^2\epsilon}[1 - 2.1035\epsilon + O(\epsilon^2)], \quad (19a)$$

$$A_{+-} = \frac{6K_4^4}{\pi^2\epsilon}[1 - 1.6647\epsilon + O(\epsilon^2)]. \quad (19b)$$

On comparing with the field-theoretical expansions of Krech [13], one finds *exact* agreement in the $O(\epsilon^{-1})$ prefactors of (19) and hence exact predictions for the contribution $\bar{A}_{+\pm}L^{-3}\ln L$ in $f^{\times}(L)$ at $d = 4$. As for the $O(\epsilon)$ terms, Krech gets 2.0987 instead of 2.1035 in A_{++} (i.e., agreement within 0.23%) and 1.6956 instead of 1.6647 in A_{+-} (agreement within 1.9%). Again, the discrepancy, although small, is larger for the $+-$ case.

To conclude, two important achievements have been reported here. First, local-functional methods have been applied to yield new quantitative predictions for critical slabs in $d = 3$. Second, by comparing with exact results in $d = 2$ and with the ϵ expansion near $d = 4$, we have demonstrated the remarkable accuracy of these methods. This adds confidence to our $d = 3$ predictions. One should also note that local functional theory has the advantage of being easily extendable to situations slightly away from the critical point.

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