Casimir Interactions in Ising Strips with Boundary Fields: Exact Results

Douglas B. Abraham[1,2] and Anna Maciołek[2,3]
[1]Theoretical Physics, Department of Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, United Kingdom
[2]Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, D-70569 Stuttgart, Germany
[3]Institute of Physical Chemistry, Polish Academy of Sciences, Department III, Kasprzaka 44/52, PL-01-224 Warsaw, Poland
(Received 26 November 2009; revised manuscript received 14 June 2010; published 26 July 2010)

An exact statistical mechanical derivation is given of the critical Casimir forces for Ising strips with arbitrary surface fields applied to edges. Our results show that the strength as well as the sign of the force can be controlled by varying the temperature or the fields. An interpretation of the results is given in terms of a linked cluster expansion. This suggests a systematic approach for deriving the critical Casimir force which can be used in more general models.

DOI: 10.1103/PhysRevLett.105.055701 PACS numbers: 64.60.fd, 05.50.+q, 64.60.an, 64.60.De

Casimir forces [1] arise in the quantum electrodynamics of confined systems, e.g., between two metal plates *in vacuo*, because the photon spectrum is modified; typically the force is attractive. Fisher and de Gennes [2] proposed that analogous Casimir forces should arise in condensed matter systems near a second-order phase transition, the agent being thermally excited fluctuations of the order parameter such as the density. Of particular interest is their scaling-theoretic prediction that such interactions should have a power law dependence on distance in the critical scaling region. For films of thickness N, the Casimir force per unit area is $\mathcal{F}_{\rm Cas} = -N^{-d}\vartheta(N/\xi)$, where ξ is the bulk correlation length and d is the spatial dimension [2–4]. (All free energies and forces are expressed in units of $k_B T$.) The scaling function ϑ depends on the universality class (UC) of a system and on the boundary conditions imposed by walls on the order parameter. ϑ was successfully measured for wetting films of helium (XY UC) [5] and of classical binary liquid mixtures (Ising UC) [6]. Recent experimental and theoretical studies show that at the submicron scale the critical Casimir force can compete successfully with other types of interactions, e.g., dispersion or (screened) electrostatic forces, in determining the properties of soft matter systems such as colloidal suspensions, liquid crystals, or fluid membranes [7]. The control of critical Casimir interactions will be crucial for many applications, e.g., in manipulating colloidal systems [8–10] or in various micro- or nanoelectromechanical devices, in particular, to be able to produce *repulsive* interactions to counteract the omnipresent attractive Casimir quantum electrodynamical force. For experimental systems belonging to the Ising UC, critical Casimir forces can be adjusted by changing temperature or boundary conditions [11]. Further, complex fluids such as liquid crystals offer more such possibilities due to the interplay between many relevant order parameters [12]. In this Letter, we derive exact partition functions for the planar Ising ferromagnet which allow the desired tunability. Second, we interpret these results as a linked cluster expansion and then indicate why it might be appropriate for more general models.

If the system is confined to a film, one would expect on intuitive grounds that the geometrical effect on the order parameter fluctuations of the strip boundaries would be to reduce the entropy, thereby establishing a strictly repulsive force. This argument is misleading, because certain aspects of the wall interactions are neglected. The first results [13] were for the strip with zero bulk field and either free boundary condition or fixed boundary spins, both the $++$ and $+-$ conditions. With $++$ and the free boundary conditions, we get attraction, but with $+-$ boundary conditions we get repulsion. Such results do not afford the desired tunability by varying parameters, but this becomes possible in a simple extension of the planar Ising model. Regarding this as a realization of a binary mixture (say), if the molecules are confined to lie in a channel, or strip, or in a membrane between two protein inclusions [14], then the energetic effects of the boundary can be approximated by surface fields or differential fugacities, as in the discussion of wetting. In addition, since electrodynamical properties

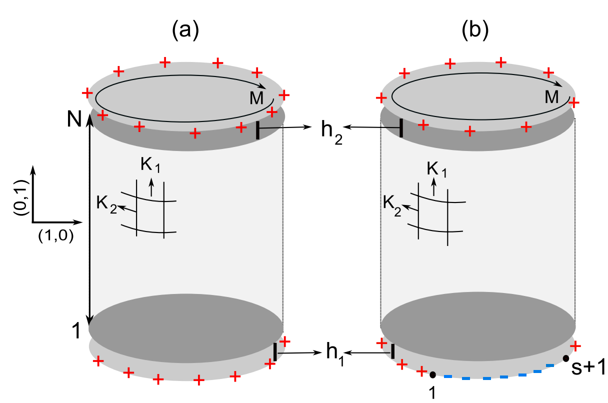

FIG. 1 (color online). Illustration of our model for (a) $h_1 h_2 > 0$ and (b) $h_1 h_2 < 0$. We are interested in the limit $M \to \infty$ with $N < \infty$. The lower boundary in (b) introduces a Peierls contour from $(1, 0)$ to $(1, s + 1)$.

of the fluid in the strip and the medium composing the walls are different, we might also include modified bonds at the surface. In this Letter, we will confine ourselves to the first case of surface fields. Our model is illustrated in Fig. 1.

The technique described in Ref. [15] allows us to calculate the partition function of a cylindrical lattice with circumference M, height N, with its axis in the $(0, 1)$ direction, and end fields $h_j > 0$, $j = 1, 2$, in a straightforward way. The fields are introduced by taking a free-edged cyclic strip and adding an extra ring of spins at each end; these spins are forced to take the value $+1$. These fixed spins are then coupled to the free lattice by bonds of strength h_1 at the bottom and h_2 at the top. A different technique, which is a finite version of the pinning-depinning, or wetting exact solution [16], is needed if $h_1 h_2 < 0$, as will be seen. The Casimir free energy for a lattice with integer coordinates at arbitrary temperature is

$$f^{\times} = -\int_{-\pi}^{\pi} \frac{d\omega}{4\pi} \ln[1 + g(\omega)e^{-2N\gamma(\omega)}], \qquad (1)$$

where $g = d^*(\omega)A_1A_2$ with $d^*(\omega) = [1 - \cos\delta^*(\omega)]/[1 + \cos\delta^*(\omega)]$ and $\gamma(\omega)$ (the Onsager function [17]) is the nonnegative solution of $\cosh\gamma(\omega) = \cosh 2K_2 \cosh 2K_1^* - \sinh 2K_2 \sinh 2K_1^* \cos\omega$ for real ω. (For clarity, in the following we will drop the explicit dependence on the argument of g and γ.) The function $\delta^*(\omega)$ is given by $e^{i\delta^*(\omega)} = [(z - A)(Bz - 1)/(Az - 1)(z - B)]^{1/2}$, where $z = e^{i\omega}$, $A = \exp 2(K_1 + K_2^*)$, and $B = \exp 2(K_1 - K_2^*)$. K_1 and K_2 are the nearest neighbor couplings in the $(0, 1)$ and $(1, 0)$ direction, respectively. K^* is the dual coupling given by the involution $\sinh(2K)\sinh(2K^*) = 1$. $A_j = (e^{-\gamma} - w_j)/(e^{\gamma} - w_j)$, $j = 1, 2$. The values w_1 and w_2 which are the wetting parameters for the force are given by [16] $w_j = e^{2K_2}(\cosh 2K_1 - \cosh 2h_j)/\sinh 2K_1$. It is crucial to note that A_j can take both positive and negative values; this is why either sign of the Casimir force is possible in principle. $++$ boundaries are obtained as a special case for $w_j = 0$, $j = 1, 2$, which gives $g = d^*$. For free boundary conditions $g = d'(\omega)$ defined by replacing δ^* by δ'; δ' has K_2 and K_1^* interchanged, which means that B^{-1} is replaced by B. This equivalence also follows from duality [15]. The Casimir force per unit length in the $(1, 0)$ direction as $M \to \infty$ has the form

$$\mathcal{F}_{\text{Cas}}(N, T) = -\int_{-\pi}^{\pi} \frac{d\omega}{2\pi} \frac{\gamma}{[1 + g^{-1}e^{2N\gamma}]}. \qquad (2)$$

Taking the scaling limit of (2), $N \to \infty$, $\gamma(0) = K_2 - K_1^* \to 0$ such that $x = N\gamma(0)\mathrm{sgn}(T - T_c)$ is fixed [as $t \equiv (T - T_c)/T_c \to 0$, $K_2 - K_1^* \simeq -4K_c t$] and $N\omega = u$, one obtains $\mathcal{F}_{\text{Cas}}(h_1, h_2, N, T) = N^{-2}\vartheta_+(\underline{r})$, with

$$\vartheta_+(\underline{r}) = -\frac{1}{\pi}\int_0^{\infty} \frac{du\,\lambda(x, u)}{\frac{X^-(0)}{X^+(0)}\frac{X_1^+X_2^+}{X_1^-X_2^-}e^{2\lambda(x,u)} + 1}, \qquad (3)$$

where $\underline{r} = (x, y_1, y_2)$ with $y_j = h_j^2 N$, $\lambda(x, u) = \sqrt{x^2 + u^2}$, and $X^{\pm}(y) = \lambda(x, u) \mp (x - 2e^{2K_c}y)$, $X_j^{\pm} = X^{\pm}(y_j)$, $j = 1, 2$. [For $T < T_c$, $\gamma(0)$ is the surface tension in the $(0, 1)$ direction of the 2D Ising model; it is the inverse correlation length for $T > T_c$.] At $x = 0$, (3) reduces to the universal Casimir amplitude, which equals $-\pi/48$ for both $h_j = 0$ and $h_j = \infty$. Interesting examples of the scaling function $\vartheta_+(\underline{r})$, which demonstrate that the critical Casimir forces can switch from attraction to repulsion by varying the temperature, are shown in Figs. 2 and 3. They were evaluated numerically from (3) for several choices of the scaling variables $y_{1,2}$. The case with $h_1h_2 < 0$ can be approached from that with $h_1h_2 > 0$ by reversing the end spins between $x = 1$ and $x = s + 1$ on one face of the cylinder, as shown in Fig. 1, thereby creating an interface with terminations in the same face. This is followed by taking the limit as $M \to \infty$, as before. With $h_j > 0$, $j = 1, 2$, we find the ratio of partition functions for strips with and without the interface to be

$$f(s) = \frac{-i}{s} \ln\int_{-\pi}^{\pi} \frac{d\omega}{2\pi} \frac{e^{is\omega}\tan(\frac{\delta^*}{2})(B^+ - B^-A_2e^{-2N\gamma})}{1 + A_1A_2e^{-2N\gamma}}, \qquad (4)$$

where $B^{\pm} = (e^{\pm\gamma} - e^{-4K_2}w_1)/(e^{\gamma} - w_1)$. If we think in the Peierls contour mode, we see that (4) can be used to define an incremental free energy associated with the dressed long contour intersecting the boundary as in Fig. 1. We are interested in the limit as $s \to \infty$ of (4) per unit length. The asymptotics for large s is dominated by the nearest singularity to the real axis in the strip $-\pi < \omega \leq \pi$. The branch cuts associated with $\sinh\gamma$ do not occur, and poles are simple zeros of the denominator of (4). Fortunately, the problem can be related to the diagonalization problem of the transfer matrix in the direction $(1, 0)$ [18] [here we are transferring in the $(0, 1)$ direction] by

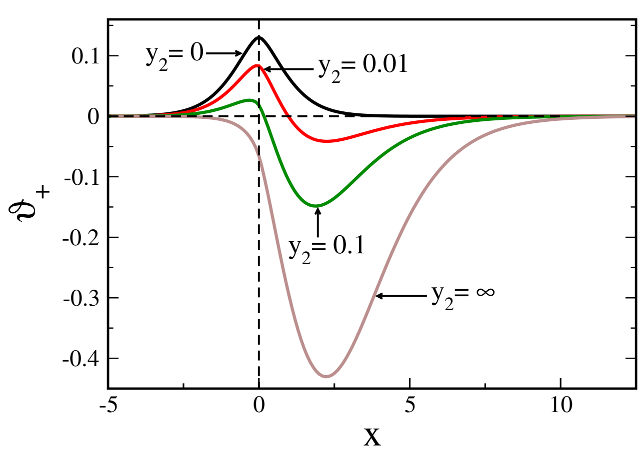

FIG. 2 (color online). The scaling function $\vartheta_+(x, y_1, y_2)$ of the critical Casimir force (3) for the isotropic lattice with $K_1 = K_2$, $x = N\gamma(0)\mathrm{sgn}(T - T_c)$, and $y_1 = h_1^2 N = \infty$ and for the several values of $y_2 = h_2^2 N$.

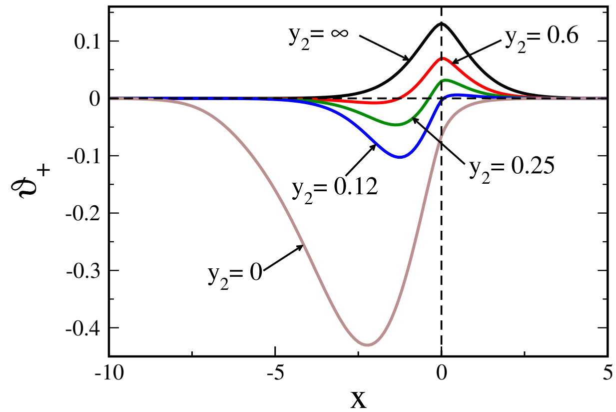

FIG. 3 (color online). The same as in Fig. 2 but with $y_1 = h_1^2 N = 0$.

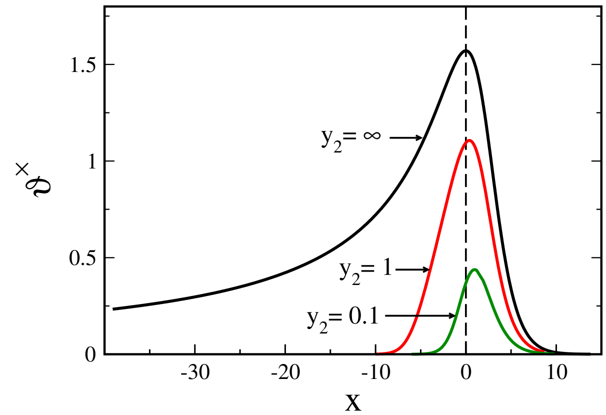

FIG. 4 (color online). The excess scaling function $\vartheta^\times(x, y_1, y_2)$ of the critical Casimir force (6) for the isotropic lattice with $K_1 = K_2$ and $y_1 = h_1^2 N = \infty$ and for the several values of $y_2 = h_2^2 N$.

looking for the solution in the variable k such that $\omega = i\hat{\gamma}(k)$ and $\lim_{\epsilon\to 0^+} \gamma[i\hat{\gamma}(k) \pm \epsilon] = \pm ik$, where the function $\hat{\gamma}(k)$ is defined as the Onsager function, but with K_1 and K_2 interchanged. Then finding zeros of the denominator of (4) becomes equivalent to solving the spectrum discretization condition for the strip transfer matrix in the $(1, 0)$ direction, which was studied in detail in Ref. [18]:

$$e^{2i(N+1)k} = e^{2i\hat{\delta}'(k)} \frac{e^{ik} w_1 - 1}{e^{ik} - w_1} \frac{e^{ik} w_2 - 1}{e^{ik} - w_2}. \quad (5)$$

$e^{i\hat{\delta}'(k)}$ is obtained from $e^{i\delta'(k)}$ by interchanging K_1 and K_2. In the scaling limit we find $f^\times = (1/N)\lambda(x, u_0)$. Hence the solution for the Casimir scaling function $\vartheta_-(\underline{r}) = \vartheta^\times(\underline{r}) + \vartheta_+(\underline{r})$ has the implicit form with

$$\vartheta^\times(\underline{r}) = \frac{u_0^2 - u_0 \underline{r} \cdot \underline{\nabla} u_0}{N^2 \lambda(x, u_0)}, \quad (6)$$

where $u_0(\underline{r})$ solves the quantization condition (5) in the scaling limit

$$e^{2iu} = -\frac{Z^+(0)}{Z^-(0)} \frac{Z_1^- Z_2^-}{Z_1^+ Z_2^+}, \quad (7)$$

where $Z_j^\pm = Z^\pm(y_j)$, $j = 1, 2$, is derived from $X_\pm(y)$ by replacing $\lambda(x, u)$ by iu. The derivatives of u_0 can be calculated straightforwardly from (7). In Figs. 4 and 5, we plot $\vartheta^\times$ as a function of x evaluated numerically for some choices of the scaling variables y_1 and y_2. Our results for the special case of $y_1 = y_2$ agree with those reported in Ref. [19]; the change of sign of the scaling function $\vartheta^\times$ is associated with the localization-delocalization transition [16,20]. This feature remains for a slightly broken symmetry, i.e., for $y_1 \approx y_2$ and $y_{1,2}$ small. For strongly asymmetric strips, the excess scaling function of the critical Casimir force is always positive.

We now interpret (1) in terms of statistical mechanical ideas. Expanding the integrand gives

$$f^\times = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \int_{-\pi}^{\pi} \frac{d\omega}{4\pi} e^{-2Nn\gamma} (C_1 C_2)^n, \quad (8)$$

where $C_j(\omega) = (A_j^-/A_j^+) \tan(\delta^*/2)$, $j = 1, 2$. Although this is not immediately apparent, this is in fact a linked cluster expansion as we now show. Equation (8) can be understood by going back to the partition function formula in terms of a transfer matrix V: $Z = \langle b_1 | V^N | b_2 \rangle$, where $|b_j\rangle$ describes the edge state with field h_j, $j = 1, 2$. Instead of using the technique described in Ref. [15], this can be developed by expanding with basis of eigenvectors of V giving

$$\frac{Z}{\Lambda_{\max}^N} = \sum_{n=0}^{\infty} \sum_{(\omega)_{2n}} \frac{e^{-N \sum_{k=1}^{2n} \gamma(\omega_k)}}{(2n)!} \langle b_1 | (\omega)_{2n} \rangle \langle (\omega)_{2n} | b_2 \rangle, \quad (9)$$

where $|(\omega)_{2n}\rangle$ denotes a $2n$-fermion eigenstate of V. This would certainly not be the chosen way of obtaining (1), since we would need to evaluate the matrix elements $\langle b_1 | (\omega)_{2n} \rangle$ and $\langle (\omega)_{2n} | b_2 \rangle$; this has been done with some

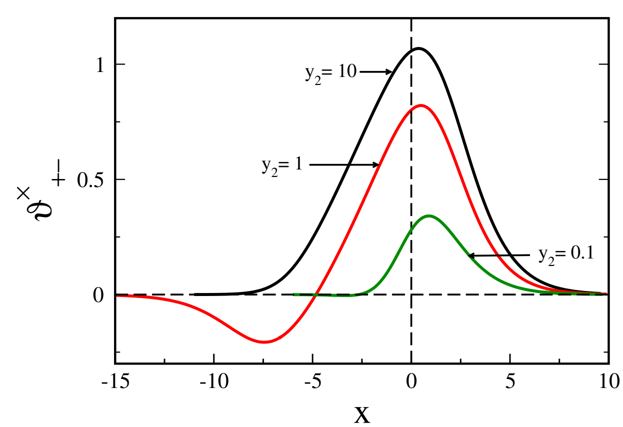

FIG. 5 (color online). The same as in Fig. 4 but for $y_1 = h_1^2 N = 1$.

effort, and the result is typically Wick-theoretic in form:

$$\langle b_j|(\omega)_{2n}\rangle = \sum_{m=2}^{2n}(-1)^m f_j(\omega_1, \omega_m)\langle b_j|\Delta_{1m}(\omega)_{2n}\rangle, \quad (10)$$

where $\Delta_{1m}(\omega)_{2n} = (\omega_2, \ldots, \omega_{m-1}, \omega_{m+1}, \ldots, \omega_{2n})$ and $f_j(\omega_1, \omega_2) = iC_j(\omega)\delta_{\omega_1, -\omega_2}$ is the contraction function or, alternatively, a scattering matrix element for a pair of fermions off the wall described by $|b_j\rangle$. Notice that, since the $A_j^{\pm}$ are even but $\tan\frac{1}{2}\delta^*$ is odd, the contraction is antisymmetric as it should be for fermions. Thus, (10) is a Pfaffian. The graphical representation of (9) and (10) is discussed in Ref. [21]. For each n we have a weighted sum of disjoint loops, each having an even number of vertices, the vertex weight $C_j(\omega)$, and the Kronecker delta edge weight. The occurrence of the Kronecker delta in the contraction function is mandated by translational symmetry. Thus, the multiple sum for each loop becomes just a single sum on implementing the deltas. Asymptotically as $M \to \infty$, each such sum is to leading order M times a single integral. We can now apply the linked cluster theorem to exponentiate (9). Equation (8) is recaptured for the excess free energy per unit length in the $(1, 0)$ direction, since the factor of $1/n$ in (8) comes directly from a symmetry number argument. Each term is then to be thought of as a weight of a "loop" with $2n$ vertices. The loop is reflected n times off the upper boundary and n times off the lower boundary, with "momentum" conservation at each reflection; thus n may be thought of as a topological quantum number. Starting from the partition function (9) and (10), we have rederived (8), in a way which allows us to identify the multiplier of $\exp(-2N\gamma)$ in (1) as a product of two scattering matrix elements, one from each edge. Clearly, γ in (9) is a fermion energy. Thus we have a complete intuitive understanding of (1). We can take the scaling limit either in (8) or (2) (as we have already done) with the same outcome. This procedure even converges after taking $T \to T_c$ in either (8) or (2), since then $\gamma(\omega) \propto |\omega|$.

Two approximation schemes are in order. First, we could consider how well partial sums of the virial series (8) approximate the exact result, so that we can assess the contribution of the different reflection number sectors to the result. Second, in the scaling limit the one-particle energy should be universal. The same is not likely to be true for the scattering matrix elements. Correlation droplet theory [22] provides an approximate method for calculating them and thus for extending the scope of our results.

In this Letter, we have described exact results for the critical Casimir force in a planar, rectangular Ising ferromagnet with applied fields h_1 and h_2 on the edges. Each field can have arbitrary sign and magnitude. Both with $h_1h_2 > 0$ and with $h_1h_2 < 0$, we show that the force can be attractive or repulsive, according to the tuning of the parameters. The compensation of attractive, quantum van der Waals forces which this will allow has implications which may well prove crucial for applications. Mean field calculations are in qualitative agreement with our results [23]. There are also related field-theoretic results [24]. We interpret the representation of the Casimir force as in (1) and (8) in terms of the linked cluster expansion. This suggest an associated droplet picture which enhances the original finite size scaling ideas of Privman and Fisher [25] in this context; this will also give new, systematic approximations for calculating critical Casimir forces in planar systems and perhaps even in $d = 3$.

D. B. A. acknowledges financial support from the Max-Planck-Gesellschaft and from the EPSRC. D. B. A. and A. M. acknowledge support and stimulation of the workshop on fluctuation-induced forces at the Kavli Institute for Theoretical Physics.

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