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Critical Casimir forces for a particle between two planar walls

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ABSTRACT

We consider a cube placed between two planar surfaces bounding a three-dimensional Ising slab. This system can be viewed as the magnetic analog of a colloidal particle immersed in a fluid, which is confined by two parallel walls. Near the bulk critical point of the Ising ferromagnet the cube gets exposed to the potential of the fluctuation that induces the critical Casimir force. Using Monte Carlo simulations we study the dependence of this potential on the relative boundary conditions at the two surfaces and at the cube within a wide range of temperatures above and below the bulk critical temperature. In order to calculate the critical Casimir force and its potential, we adopt an approach based on an integration scheme of free energy differences. The scaling functions of the corresponding critical Casimir forces are also determined.

1. Introduction

Two objects immersed in a fluid which is brought to its bulk critical point T_c experience the so-called critical Casimir interaction [1]. This effective interaction arises due to modifications of the structure of the fluid and due to the restrictions of the fluctuation spectrum of its order parameter by the surfaces of the objects. Accordingly, not only the temperature T but also the adsorption properties of both objects and their geometry determine the sign, the strength and the range of the critical Casimir forces (CCFs). In asymptotic regimes ($T \to T_c$ and all distances large compared with microscopic lengths) finite-size scaling [2] holds and the CCFs are described by universal scaling functions. Universality permits to use the simplest possible representative of the same universality class in order to calculate these scaling functions. In this sense the Ising model represents systems such as simple one-component fluids or binary liquid mixtures.

The simple geometry of two parallel planes can be realized experimentally by growing a wetting film; exactly the wetting films were used to provide first reliable evidence for the existence of the CCFs [3–6]. On the other hand, even for this simple geometry determination of the scaling functions from corresponding model systems is a challenging task. Theoretical approaches which incorporate critical fluctuations beyond the Gaussian approximation and can take into account a dimensional crossover occurring in films are intractable for most of the relevant experimentally boundary conditions (BCs). Monte Carlo (MC) simulations offer a very useful alternative approach, which is however not free from difficulties. Within this approach the range of sizes of the system is strongly limited by the steeply increasing computational costs. For the thicknesses and the aspect ratios of slabs accessible in simulations, numerical data do not collapse and corrections to scaling are necessary. Renormalization-group analyses reveal that there is a whole variety of sources for corrections to scaling which arise from bulk, surface, and finite-size effects [2]. In addition to the leading bulk corrections to scaling (with the correction-to-scaling exponent $\omega \simeq -0.8$) one expects corrections due to the finite aspect ratio, corrections due to the boundary conditions (which are especially large for the symmetry breaking boundary conditions) and, moreover, next-to-leading corrections might occur for narrow films. In spite of these difficulties the Casimir scaling functions in three spatial dimensions ($3d$) have been obtained rather accurately for experimentally relevant universality classes with a variety of BCs and surface fields [7–14].

In the present paper we study numerically the CCFs acting on a cube located between two planar walls as a function of temperature and separation for different BCs. The cube mimics a colloidal particle positioned near the wall. We use MC simulations of the Ising model on a cubic lattice as a representative of the Ising universality class of critical phenomena. The aim of this work is twofold. We would like to check whether the approach that we used in our previous studies for a slab geometry [8–11] can be successfully adopted for the present geometry. This approach is based on the so-called coupling parameter method where the difference of free energies is expressed as an integral over the mean energy difference (see, e.g., Refs. [8] and [15]). Moreover, we address the question of the mechanical stability of a cube particle for the cases when (a) both walls and the particle have the same adsorption preference (+| + |+), (b) the walls have opposite adsorption preferences (+| + |−), and (c) the cube particle is

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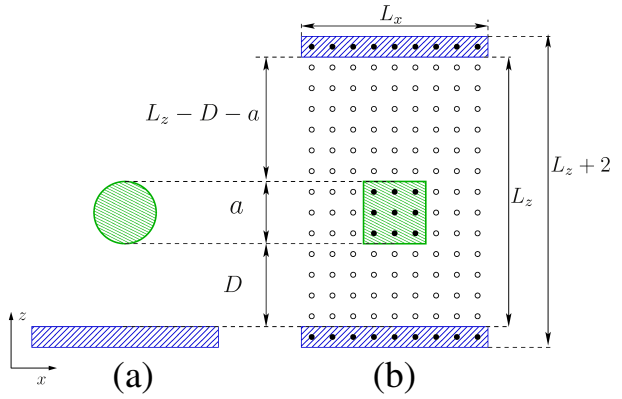

Fig. 1. The geometry under consideration (the cross-section in the xz plane): (a) the spherical particle of the diameter a at the distance D from the wall; (b) an appropriate geometry on the lattice for a cubic particle with the edge length a at the separation D from the bottom wall. The total system size is $L_x \times L_y \times (L_z + 2)$, and the separation of the particle from the top wall is $L_z - D - a$, where L_z is the number of layers of free spins.

neutral and the walls have opposite adsorption preferences $(+|0|-)$. These situations can be mimicked in our Ising system by choosing an appropriate BC on the lattice sites forming boundaries of the three objects. Because of unavoidable limitations of the size of the system, we cannot expect to reach the asymptotic region of the universal behavior in our simulations. Nevertheless, after rescaling procedure for some BCs we have obtained a reasonable data collapse.

Recently, a different MC simulation method for spin models which mimic the sphere–planar plane geometry has been developed [16]. The geometry of a sphere or a cube near a *single* planar surface is relevant for colloidal systems or in experimental setups of high-precision force measuring devices and methods, such as atomic force microscope (AFM) [17], surface force apparatus (SFA) [18] or total internal reflection microscopy (TIRM) [19,20]. For this geometry theoretical predictions for the CCFs are much more limited than for films. The MC simulation method employed in Ref. [16] is similar to the one used in [7] for the plate–plate geometry, where differences of the free energy are computed by integrating differences of the energy over the inverse temperature. Simulations have been performed for the improved Blume–Capel model on the simple cubic lattice, which shares the universality class of the three-dimensional Ising model but has the advantage over it that the amplitudes of the leading correction to scaling are substantially suppressed. The focus of that study was on symmetry breaking boundary conditions at the surfaces of the sphere and the plate. The use of the geometric cluster algorithm and the introduction of an effective radius of the sphere and the effective distance from the wall have allowed the author to obtain a good data collapse. Still another MC simulation method to compute the critical Casimir force acting between the disk and the wall in two-dimensional Ising systems has been proposed in Ref. [21]. This method is analogous to the one used in experiments reported in Refs. [19,20] for a colloidal particle where the Casimir potential is determined from the distribution of the position of the particle above the wall. The interaction between two particles in the presence of the bulk ordering field recently has been studied by using a local field integration method [22].

Our presentation is organized as follows. In Section 2 we briefly present the relevant theoretical background, introduce our model, and describe the numerical method employed in order to compute the CCFs and its scaling functions from the MC simulation data. Section 3 contains our results. We provide a summary and conclusions in Section 4.

2. The model and the method

2.1. Theoretical background

Let us consider a spherical colloidal particle of a diameter a immersed in critical binary mixture near a wall, see Fig. 1(a).

As already mentioned in the Introduction, at the critical point of the demixing transition of the binary solvent, the CCFs, which are the analogs of the electromagnetic Casimir force [23], emerge between the wall and the colloidal particle as a result of critical fluctuations of the order parameter of the solvent and the critical adsorption of a preferable component of the mixture on the surfaces of wall and the colloid. For a binary mixture the order parameter is the deviation of the concentration of the one component of the mixture from its value at the critical point. The CCFs between the wall and the particle are obtained from the free energy $U_C(\beta, D, a)$ of a system consisting of the colloidal particle of the characteristic linear size a immersed in the fluid at the inverse temperature $\beta = 1/k_BT$ at the separation D from the planar wall:

$$f_C(\beta, D, a) = -\frac{\partial U_C(\beta, D, a)}{\partial D}. \tag{1}$$

Note that the above definition of the CCFs differs from the one used to define the CCFs between two planar parallel plates immersed in the

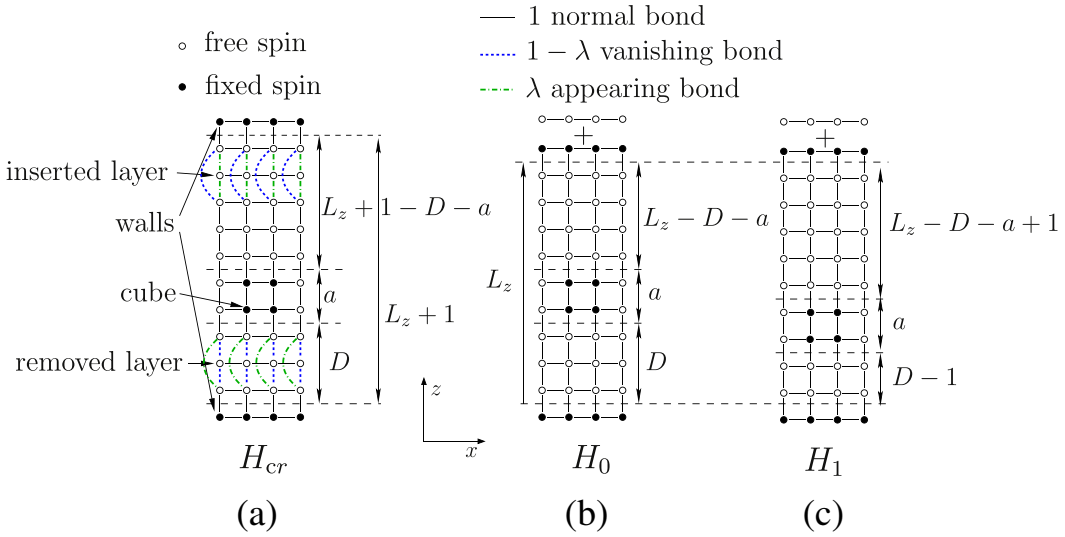

Fig. 2. Bond arrangement for the computation of the free energy difference in Eq. (9) (see main text). The crossover Hamiltonian H_{cr} (a) describes the system which interpolates between those described by the Hamiltonians H_0 (b) and H_1 (c).