Critical Casimir forces for various boundary fields obtained by Monte Carlo simulation: crossover from repulsion to attraction

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The confinement of concentration fluctuations in binary liquid mixtures close to the bulk critical point generates long-ranged forces acting on the confining surfaces. In analogy with the quantum Casimir forces which are induced by vacuum fluctuations of the electromagnetic field, the forces in critical liquids are called *critical Casimir forces*. During the last two decades these phenomena have been studied experimentally, theoretically, and numerically for binary liquid mixtures (Ising model universality class) and for liquid He^4 and He^3–He^4 mixture (XY model universality class).

We have studied critical Casimir forces in 3D Ising films with surface fields by using Monte Carlo simulations. The critical Casimir force in a film of thickness L with surface fields H_1 scales as $\beta f_{\rm Cas}(T, L, H_1) = L^{-d}\theta_{\rm Cas}(L/\xi, h_1)$ where $\theta_{\rm Cas}(L/\xi, h_1)$ is a universal scaling function, ξ is the bulk correlation length, and $h_1 = H_1 L^{\Delta_1/\nu}$ is the scaling variable associated with the surface field. Here ν and Δ_1 are the correlation length and surface field critical exponents, respectively.

A numerical method based on an integration scheme for the free energy differences is used to compute the universal Casimir forces in the critical region for the Ising model for various values of the boundary fields. We study the scaling of the Casimir force as function of L/ξ and h_1 taking into account finite size corrections to scaling. We pay special attention to that region of the surface field H_1 where the force changes from repulsion to attraction upon increasing the temperature. Our results are compared with corresponding experimental data for wetting films of fluids as well as with other available theoretical results.