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Critical Casimir forces from the equation of state of quantum critical systems

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The mapping between a classical length and inverse temperature as imaginary time provides a direct equivalence between the Casimir force of a classical system in D dimensions and internal energy of a quantum system in $d = D - 1$ dimensions. The scaling functions of the critical Casimir force of the classical system with periodic boundaries thus emerge from the analysis of the symmetry related quantum critical point. We show that both nonperturbative renormalization group and quantum Monte Carlo analysis of quantum critical points provide quantitative estimates for the critical Casimir force in the corresponding classical model, giving access to widely different aspect ratios for the geometry of confined systems. In light of these results, we propose protocols for the realization of critical Casimir forces for periodic boundaries through state-of-the-art cold-atom and solid-state experiments.

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Introduction. The behavior of a system close to a second-order phase transition is described by universal scaling functions, independent of the microscopic details of the system, the study of which is a challenge to both experiments and theory. In this context, a uniquely accessible universal feature is represented by the critical Casimir force, which has been the object of an impressive amount of experimental [1–4], theoretical [5–7], and numerical work [8–11]. At a phase transition, diverging order parameter fluctuations lead to a force on confining boundaries which impose a spatial cutoff of correlations along one spatial dimension [12], in a way formally similar to the Casimir effect [13] in quantum electrodynamics. The dependence of the force on the confinement length and on the distance to the critical point is governed by a universal scaling function characteristic of the bulk and the surface universality classes, and whose sign and scale depend crucially on the boundary conditions (BCs) [14,15].

In the realm of critical phenomena, one of the most active subjects across the physical spectrum (from high-energy physics, to condensed matter, to cold atoms, etc.) is the study of quantum critical points (QCPs), i.e., zero-temperature phase transitions of quantum systems [16]. Our understanding of quantum many-body systems in general, and of QCPs in particular, often relies on the quantum-to-classical mapping provided by the functional integral description of quantum statistical physics, by which a d-dimensional quantum system at $T = 0$ is represented as an effective classical system in $D = d + 1$ dimensions with periodic BCs in the extra, imaginary-time dimension [see Figs. 1(a) and 1(b)]. This mapping underlies our understanding of a many zero-temperature QCPs in relationship with thermal critical points in $d + 1$ dimensions.

In this Rapid Communication we turn this paradigm on its head, showing that the mapping to quantum transitions can provide different insight into thermal transitions. Indeed, turning on a finite temperature close to a QCP amounts to introducing a finite length (with periodic BCs) to the extra dimension of the effective classical theory, so that the critical Casimir force for a classical system with periodic BCs appears naturally [17]. In particular, we show that the thermal energy of the quantum system plays the same role as the critical Casimir force of the classical system, as they are described by the same universal scaling function [Fig. 1(c)]. This mapping allows us to turn the considerable arsenal of field theoretic and numerical tools developed for the QCP towards the critical Casimir scaling function. We show that the nonperturbative renormalization group (NPRG) and the quantum Monte Carlo (QMC) approach can provide estimates for the scaling function of three-dimensional $O(N)$ spin models, where N is the number of components of the order parameter, with precision and flexibility which, in the case of the NPRG, are remarkable for theoretical methods. Moreover, this insight highlights the fact that the thermal energy of a quantum system in the vicinity of a QCP is a universal

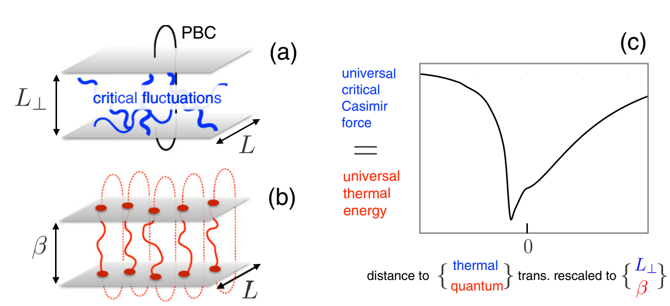

FIG. 1. The central theme of this work is the correspondence between (a) D-dimensional classical critical phenomena in confined geometries with periodic boundary conditions (PBCs), and (b) quantum many-body systems in $d = D - 1$ dimensions at finite temperature and close to a quantum critical point. (c) Our main result is that the critical Casimir force of the classical system is described by the same universal scaling function as the thermal energy of the quantum system.

TABLE I. Conversion table between classical and quantum critical systems. t is the reduced temperature of the classical system and δ the nonthermal control parameter of the quantum phase transition.

Classical	D	$L_\perp$	t	ξ	Casimir force
Quantum	$d+1$	$\beta\hbar c$	δ	ξ,ξ_τ	Internal energy

scaling function, which is potentially accessible to a variety of state-of-the-art experiments on complex quantum systems.

Classical versus quantum scaling functions. We consider a D-dimensional classical system with thickness $L_\perp$ and cross-sectional area L^{D-1}, which, in the thermodynamic limit, $L,L_\perp \to \infty$, undergoes a second-order phase transition at a temperature T_c. The free energy can be written as [18]

$$\Omega(t,L,L_\perp) = L^{D-1}L_\perp k_BT[\omega_{\rm ex}(t,L,L_\perp) + \omega_{\rm bulk}(t)], \quad (1)$$

where $t=(T-T_c)/T_c$ is the reduced temperature. Here, $\omega_{\rm bulk}$ denotes the free-energy density in the thermodynamic limit, in units of k_BT, and $\omega_{\rm ex}$ the "excess" contribution due to the finite volume of the system. For $D<4$, hyperscaling implies that the excess free-energy density can be written in the scaling form [19]

$$\omega_{\rm ex}(t,L,L_\perp) = L_\perp^{-D}\mathcal{F}_\pm\left(\frac{L_\perp}{\xi},\frac{L_\perp}{L}\right), \quad (2)$$

where $\mathcal{F}_\pm$ is a universal scaling function which depends only on the universality class of the (bulk) phase transition and the boundary conditions. The $+/-$ index refers to the disordered ($T>T_c$) and ordered ($T<T_c$) phases, respectively. The correlation length $\xi=\xi_{0\pm}|t|^{-\nu}$ diverges at the transition with a critical exponent ν. In the low-temperature phase, when the spontaneously broken symmetry is continuous, ξ should be interpreted as the Josephson length, i.e., the length separating long-wavelength (gapless) Goldstone modes from critical fluctuations at shorter length scales [20]. The scaling form (2) holds whenever ξ, L, and $L_\perp$ are much larger than the Ginzburg length ξ_G (scaling limit) [16].

The Casimir force per unit area, in units of k_BT, is then [21,22]

$$f_C(t,L,L_\perp) = L_\perp^{-D}\vartheta(x,y) = -\frac{\partial}{\partial L_\perp}L_\perp\omega_{\rm ex}(t,L,L_\perp), \quad (3)$$

where the choice of scaling variables, $x=t(L_\perp/\xi_{0+})^{1/\nu}$ and $y=L_\perp/L$, allows for the definition of a single universal scaling function above and below the transition [$\omega_{\rm ex}=L_\perp^{-D}\mathcal{F}(x,y)$]:

$$\vartheta(x,y) = (D-1)\mathcal{F}(x,y) - \frac{x}{\nu}\frac{\partial\mathcal{F}(x,y)}{\partial x} - y\frac{\partial\mathcal{F}(x,y)}{\partial y}. \quad (4)$$

The scale of the force is determined by $\vartheta(0,y)$, the value at the critical point. This amplitude passes through zero for $y=1$ and diverges as $y\to\infty$ [22]. It is thus useful, for $y>1$, to define $f_C=L^{-D}\tilde\vartheta$, such that the scaling function $\tilde\vartheta(x,y)=y^{-D}\vartheta(x,y)$ has a finite limit for $x=0$ and $y\to\infty$.

The scaling function ϑ being universal, it is independent of the details of the microscopic interactions and is fully determined by the space dimension D, the nature of the order parameter, the range of the interactions, and the boundary conditions. ϑ can therefore be computed from a field theory. For short-range interactions, the latter can be defined through the functional integral $Z=\int\mathcal{D}[\boldsymbol{\varphi}]\exp(-\beta H)$ for the partition function and the (local) Hamiltonian

$$\beta H = \int_{L^{D-1}} d^{D-1}r_\parallel \int_0^{L_\perp} dr_\perp\, \mathcal{H}(\boldsymbol{\varphi},\boldsymbol{\nabla}_\parallel\boldsymbol{\varphi},\partial_\perp\boldsymbol{\varphi};\{g_i\}), \quad (5)$$

where the integration over $\mathbf{r}_\parallel$ is restricted to the area L^{D-1}. $\boldsymbol{\varphi}(\mathbf{r}_\parallel,r_\perp)$ denotes the N-component order parameter field and $\{g_i\}$ a set of coupling constants (we distinguish between parallel and perpendicular gradient terms, $\boldsymbol{\nabla}_\parallel\boldsymbol{\varphi}$ and $\partial_\perp\boldsymbol{\varphi}$, for later convenience). The dimensionless free energy, $\beta\Omega=-\ln Z$, where $\beta=1/k_BT$, depends on temperature through the (usually phenomenological) coupling constants of the classical field theory. For simplicity, we consider in the following homogeneous and isotropic classical systems.

To any such D-dimensional field theory defined in a volume $L^{D-1}L_\perp$ with periodic boundary conditions in the perpendicular direction, one can associate a quantum field theory in $d=D-1$ space dimensions by identifying $L_\perp\equiv\beta\hbar c$, where c is a characteristic velocity and where the spatial coordinate $r_\perp\equiv c\tau$ relates to an imaginary time τ. The Hamiltonian of the classical theory maps onto the (Euclidean) action of the quantum field theory,

$$S = \int_0^{\hbar\beta} d\tau \int_{L^d} d^dr\, \mathcal{H}(\boldsymbol{\varphi},\boldsymbol{\nabla}\boldsymbol{\varphi},\partial_\tau\boldsymbol{\varphi};\{g_i\}), \quad (6)$$

where the g_i's are now temperature independent. Although βH and S are formally identical (up to a change in notations), they describe different physical systems. The Hamiltonian H describes a D-dimensional classical system which undergoes a thermal phase transition in the thermodynamic limit $L,L_\perp\to\infty$. The action S describes a d-dimensional quantum system which, in the thermodynamic limit $L\to\infty$, undergoes a zero-temperature phase transition where both the correlation length $\xi=\tilde\xi_{0,\pm}|\delta|^{-\nu}$ and the time scale $\xi_\tau=\xi/c$ diverge, and the critical modes at the QCP have a linear dispersion, $\omega=c|\mathbf{q}|$, corresponding to the dynamical exponent $z=1$ [16]. This transition is driven by a nonthermal parameter δ, assumed here to vanish at the QCP, which enters in S only through the (usually phenomenological) δ dependence of the coupling constants g_i.

The critical point described by the classical field theory and the QCP described by the quantum field theory are formally equivalent and fall in the same universality class. A finite area L^{D-1} in the classical model corresponds to a finite volume L^d in the quantum model, and a finite thickness $L_\perp$ to a nonzero temperature T. The scaling analysis of the classical model straightforwardly translates to the quantum model. From Eqs. (1) and (2), we obtain the free energy

$$\Omega(\delta,L,T) = \Omega_{\rm bulk} + L^d\frac{(k_BT)^{d+1}}{(\hbar c)^d}\mathcal{F}(x,y), \quad (7)$$

where $\Omega_{\rm bulk}=L^d\epsilon_{\rm gs}(\delta)$ is the zero-temperature bulk contribution, proportional to the ground-state energy density $\epsilon_{\rm gs}$. The scaling variables are now $x=\delta(\beta\hbar c/\tilde\xi_{0,+})^{1/\nu}$ and $y=\beta\hbar c/L$.

The internal energy density $\epsilon = L^{-d}\partial(\beta\Omega)/\partial\beta$ is given by

$$\epsilon(\delta,L,T) = \epsilon_{\rm gs}(\delta) - \frac{(k_BT)^{d+1}}{(\hbar c)^d}\vartheta(x,y), \tag{8}$$

where ϑ is the universal scaling function of the critical Casimir force defined in Eq. (4). Comparing Eqs. (3) and (8), we see that the Casimir force provides a measure of the difference between $\epsilon_{\rm gs}$ and $\epsilon(\delta,L,T)$. Notably, taking the thermodynamic limit, $L \to \infty$ ($y = 0$), one can deduce from this analysis, without prior knowledge, that the critical Casimir force of the classical system in slab geometry is negative, given that in this limit $-\vartheta$ is proportional to the thermal energy, which is always positive. The situation for general y is discussed further below. A summary of the conversion from the classical to the quantum terminology is given in Table I.

Renormalization group calculation of the critical Casimir force in $O(N)$ models. Previous theoretical studies of the critical Casimir force with periodic boundary conditions have concentrated on the large N expansions and the ϵ expansion close to four dimensions. The former allows analytic calculations over the whole phase diagram, but fails to catch the nonmonotonous shape at finite N of the scaling function for periodic boundary conditions [5]. In the case of the ϵ expansion, it typically fails in the ordered phase, and converges poorly at the critical point [6,7]. Here, we use the NPRG to compute the scaling function ϑ in the context of the two-dimensional quantum $O(N)$ model, defined by the action

$$S = \int_0^{\hbar\beta} d\tau \int d^2r \left\{ \frac{(\nabla\boldsymbol{\varphi})^2}{2} + \frac{(\partial_\tau\boldsymbol{\varphi})^2}{2c^2} + \frac{r\boldsymbol{\varphi}^2}{2} + \frac{u(\boldsymbol{\varphi}^2)^2}{4!} \right\}, \tag{9}$$

where $\boldsymbol{\varphi}$ is an N-component real field satisfying periodic boundary conditions $\boldsymbol{\varphi}(\mathbf{r},\tau+\hbar\beta) = \boldsymbol{\varphi}(\mathbf{r},\tau)$. r and u are temperature-independent coupling constants and c is the (bare) velocity of the $\boldsymbol{\varphi}$ field. The QCP at $r = r_c$ ($\delta = r - r_c$ for this model) is in the universality class of the three-dimensional classical $O(N)$ model, and the phase transition is governed by the three-dimensional Wilson-Fisher fixed point.

The renormalization group is a natural approach to compute universal quantities in the (quantum) $O(N)$ model. The calculation of scaling functions of the (2+1)-dimensional Wilson-Fisher fixed point is, however, notoriously difficult and perturbative renormalization group usually fails. In the following, we show that the NPRG provides us with a scaling function of the critical Casimir force which compares very well with results obtained from Monte Carlo simulations of three-dimensional classical spin systems (see also Ref. [23]). We only consider the thermodynamic limit, i.e., $L \to \infty$, and thus the scaling function $\vartheta(x,0)$.

The NPRG is an implementation of the Wilsonian RG based on an exact equation for the Gibbs free energy (or "effective action" in field theory terminology) for which powerful approximation schemes have been designed [24–26]. Recently, the NPRG has been used to study the thermodynamics of the quantum $O(N)$ model [27], the Higgs amplitude mode [28,29] (in very good agreement with Quantum Monte-Carlo simulations [30]), the quantum-to-classical crossover in the dynamics [31], and the Kosterlitz-Thouless transition in the two-dimensional $O(2)$ model [32–34]. Our results, which are exact in the limit $N \to \infty$, are obtained from a derivative expansion of the effective action to second order and improves on the approach of Ref. [27] (see the Supplemental Material for more details [35]).

Figure 2 shows the Casimir scaling function ϑ obtained from the two-dimensional quantum $O(N)$ model within the NPRG approach for the three-dimensional Ising ($N = 1$), XY ($N = 2$), and Heisenberg ($N = 3$) universality classes, together with data from Monte Carlo simulations of the three-dimensional classical spin systems [8,22,36,37]. In all cases we find very good agreement between the NPRG and simulation results. In particular, the nonmonotonous form for $\vartheta(x,0)$ is well reproduced and the amplitude and position of the minimum of the scaling function are accurately predicted, with some small differences between NPRG and simulations occurring in the region around $x \simeq -1$, with the former showing a more pronounced minimum for $N = 1$ and $N = 2$. Note that in Ref. [37], the overall scale of the $N = 3$ scaling function was not determined. We have rescaled the MC data so that they satisfy the known asymptotic value when $x \to -\infty$, $-2(N-1)\zeta(3)/2\pi$, corresponding to the excess free energy of bosons with linear dispersion [27]; the rescaled function compares well with the NPRG result.

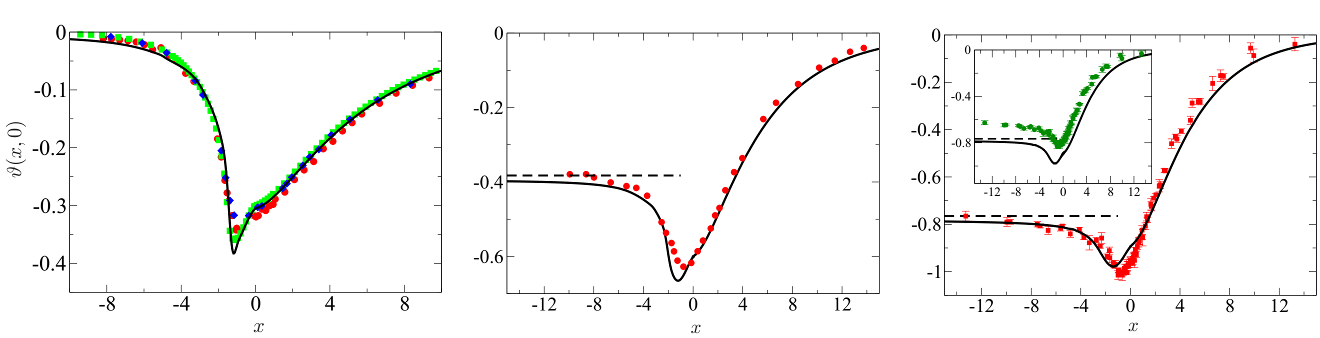

FIG. 2. Casimir scaling function $\vartheta(x,0)$ for the three-dimensional $O(N)$ universality class from the NPRG approach to the two-dimensional quantum $O(N)$ model (solid line), compared to classical Monte Carlo simulations of the corresponding three-dimensional spin models (symbols). The horizontal dashed line shows the (exact) limit $-2(N-1)\zeta(3)/2\pi$. Left panel: Ising ($N = 1$) universality class. Monte Carlo simulations are from Ref. [8] (blue diamonds), Ref. [22] (green squares), and Ref. [36] (red circles). Middle panel: XY universality class ($N = 2$). The Monte Carlo data are from Ref. [8]. Right panel: Heisenberg universality class ($N = 3$). The Monte Carlo data [37] have been rescaled so as to satisfy the correct asymptotic value for $x \to -\infty$ (see text); the bare data are shown in the inset.

TABLE II. Universal Casimir amplitude $\vartheta(0,0)/2$.

N	1	2	3
NPRG	−0.1527	−0.3006	−0.4472
Monte Carlo [8]	−0.1520(2)	−0.2993(7)	

We show in Table II the NPRG and Monte Carlo estimates for the universal Casimir amplitude $\vartheta(0,0)/2$. Again, the NPRG results are in very good agreement with MC simulations, with a relative difference below 1% [38].

Finite-size scaling and aspect ratio. The method of choice for a fully quantitative study of a QCP is QMC. It provides the flexibility to vary the spatial as well as the time dimension, allowing for the evolution from slab to column geometry in the corresponding classical system through the variation of the ratio $y = \beta\hbar c/L$. As a consequence, the standard finite-size and finite-temperature scaling analysis of the numerical results close to the quantum critical point can be recast in the language of critical Casimir forces in columnar geometry [17]. Indeed, the finite nature of the simulation cell implies that the quantum limit, $\beta \to \infty$, corresponds to column geometry for the corresponding classical system. With continuous-time QMC [39], the imaginary-time axis becomes a continuous periodic dimension of length $\beta\hbar c$, as in the field theoretic approach, so that y can be easily tuned to any value. Furthermore, the internal energy $\epsilon = L^{-d}\langle\hat{H}\rangle$, where $\hat{H}$ is the Hamiltonian of the quantum system, is an easily accessible observable, whereas the numerical methods for calculating the Casimir force in classical systems are computationally intensive [8,10,22,40]. Following Eq. (8), one can fit the numerical calculation for energy density $\epsilon(\delta,L,T)$ to a suitable scaling function (this kind of fit has been used to compute $\tilde{\vartheta}$ in the limit $y \gg 1$ for quantum systems [41,42]).

We have studied the quantum critical point of the transverse-field Ising model in two dimensions, $\hat{H} = -J\sum_{\langle i,j\rangle}\hat{\sigma}_i^z\hat{\sigma}_j^z - h\sum_i\hat{\sigma}_i^x$, which has a QCP at $h = h_c$ ($\delta = h - h_c$ here) between a ferromagnetic and a paramagnetic ground state. We have used a cluster QMC algorithm [43] to compute the energy density, while the critical velocity c is extracted from the excitation spectrum at the QCP [44] (see the Supplemental Material [35]). Numerical results for the critical Casimir amplitude estimated from QMC over the range $0 < y < \infty$ are shown in Fig. 3 and compared with classical simulation results for the three-dimensional Ising model from Ref. [22]. Excellent agreement is found, confirming the equivalence of these two critical phenomena away from the limit of slab geometry. There is a sign change at $y = 1$: For $y \ll 1$, $-\vartheta$ probes the (positive-definite) thermal energy density, whereas for $y \gg 1$ it probes the finite-size corrections to the ground-state energy density, which are usually negative for quantum systems.

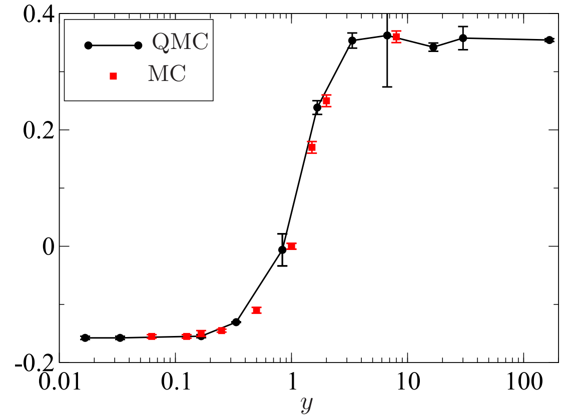

FIG. 3. Evolution of the Casimir amplitude extracted using QMC from the quantum Ising model as a function of the aspect ratio y. We show $\vartheta(0,y)/2$ for $y \leqslant 1$ and $\tilde{\vartheta}(0,y)$ for $y \geqslant 1$. Red squares are classical Monte Carlo (MC) data from Ref. [22].

Conclusion. The finite-temperature equation of state for a quantum critical system in dimension d can in principle be measured in state-of-the-art experiments on quantum critical phenomena, including trapped ions [45] and quantum Ising magnets in a transverse field [46] for $N = 1$, ultracold Bose gases loaded in optical lattices for $N = 2$ [47], and quantum magnets under pressure for $N = 2$ and $N = 3$ [48]. The critical Casimir force for a classical system in dimension D with a thermal critical point could hence be experimentally accessed, opening the door to a different class of critical Casimir force experiments in which the quantum system becomes a simulator for confinement effects on critical fluctuations at a classical critical point. Conversely, the interpretation of the thermal energy as a critical Casimir force challenges the experiments on quantum critical phenomena to measure the corresponding universal scaling function. This can be achieved in the solid-state context via temperature integration of the specific heat, and in the atomic physics context by direct measurement of spin-spin or density-density correlation functions for the potential part, and by time-of-flight measurement for the kinetic part. The above considerations exhibit the as yet unexplored potential of the quantum-to-classical correspondence in the context of critical phenomena.

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