Evidence for Fisher Renormalization in the Compressible ϕ^4 Model

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We present novel Fourier Monte Carlo simulations of a compressible ϕ^4-model on a simple-cubic lattice with linear-quadratic coupling of order parameter and strain, focusing on the detection of fluctuation-induced first-order transitions and deviations from standard critical behavior. The former is indeed observed in the constant stress ensemble and for auxetic systems at constant strain, while for regular isotropic systems at constant strain, we find strong evidence for Fisher-renormalized critical behavior and are led to predict the existence of a tricritical point.

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A proper treatment of strain effects is absolutely essential for understanding phase transitions in real solids. Despite extensive efforts made in clarifying the role of elasticity in affecting phase transitions, the existing literature reveals quite a bit of persistent controversy [1–3], which also hints at the great difficulty of questions posed by these systems equally to theorists, experimentalist, and computer simulators alike. Theoretical analysis, most of which took place during the dawn [4,5], the boom years [6,7] of the renormalization group (RG), indicates that many different situations (boundary conditions, anisotropy, symmetry and strength of coupling between primary order parameter and strain) must be carefully distinguished. This leads to a wealth of predictions of various phase transitions of first or second order with bare or Fisher-renormalized [5] critical exponents. Experimentally, however, finite temperature resolution, defect smearing, and other effects can make it quite difficult to distinguish possibly second from weakly first-order transition, while computer simulations are fundamentally challenged by the long-range strain effects. To illustrate the difficulties, consider a ϕ^4-model with spins $s(\boldsymbol{x})$ coupled in a quadratic-linear way to a fluctuating strain field ϵ_{ij} built from six homogeneous strain components and the spatial derivatives of a real-valued displacement vector field, governed by the Hamiltonian [7]

$$\mathcal{H}[s,\epsilon] = \int_V d^3x \Big(\frac{D}{2}(\nabla s)^2(\boldsymbol{x}) + \frac{A_2}{2} s^2(\boldsymbol{x}) + \frac{A_4}{4} s^4(\boldsymbol{x}) + g_0 s^2(\boldsymbol{x}) \sum_i \epsilon_{ii}(\boldsymbol{x}) + \frac{1}{2} \sum_{ijkl} C^0_{ijkl} \epsilon_{ij}(\boldsymbol{x}) \epsilon_{kl}(\boldsymbol{x}) \Big). \tag{1}$$

In a MC simulation of a discretized approximation to this model, one basically has two choices, which, from the point of view of real-space algorithms, are equally unattractive. If the elastic degrees of freedom are kept explicitly, the inhomogeneous components of a strain tensor field and the accompanying elastic energy have to be recalculated at every move, which is time consuming. On the other hand, an exact elimination of the elastic degrees of freedom, which only enter harmonically into the above Hamiltonian by Gaussian integration, leaves us with an effective Hamiltonian

$$\mathcal{H}_{\text{eff}}[s] = \int_V d^3x \Big(\frac{D}{2}(\nabla s)^2(\boldsymbol{x}) + \frac{A_2}{2} s^2(x) + \frac{A_4}{4} s^4(\boldsymbol{x}) \Big) - \int d^3x d^3y s^2(\boldsymbol{x}) \mathcal{K}(\boldsymbol{x}-\boldsymbol{y}) s^2(\boldsymbol{y}). \tag{2}$$

Compared to the incompressible ϕ^4 Hamiltonian, the fourth order coupling coefficient A_4 displays a renormalization by a complicated nonlocal term. In terms of its Fourier transform $\tilde{\mathcal{K}}(\boldsymbol{k}) = \sum_{ij} \tilde{\mathcal{K}}_{ij}(\boldsymbol{k})$, this term can be calculated from summing over the components of the tensor function

$$\tilde{\mathcal{K}}_{ij}(\boldsymbol{k}) = \begin{cases} g_0^2 \kappa_0, & \boldsymbol{k} = \boldsymbol{0} \\ g_0^2 (D^0)^{-1}_{ij}(\boldsymbol{k}) k_i k_j, & \boldsymbol{k} \neq \boldsymbol{0} \end{cases} \tag{3}$$

which is in turn built from the inverse of the (bare) dynamical phonon matrix $D^0_{ik}(\boldsymbol{k}) = \sum_{jl} C^0_{ijkl} k_j k_l$. It thus comes as no surprise that, as far as the author knows, it is only in the case of elastic isotropy in cubic systems (see below) that a relatively compact and simple real-space representation of this Hamiltonian that lends itself to a real-space MC algorithm can be derived [2]. In general, the nonlocal character of this interaction, which reflects the long-range strain interaction, renders this effective Hamiltonian useless in designing real-space MC algorithms. An alternative route (cf., e.g., Ref. [3]) is to represent the elastic interactions by pair, triple, and four-spin interactions using effective interaction potentials like the Stillinger-Weber potential. Unfortunately, using such approaches, the elastic behavior of the system is much harder to control than by, say, imposing a set of "bare elastic constants" on the system right from the start. In particular, one regrets the lack of control of elastic anisotropy, which, while certainly found in most real systems, is a crucial quantity in theoretical calculations [7]. Not unlike in a real-world experiment, an additional concern is the distinction of weak first-order from truly continuous phase transitions.

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In principle, this can be done using finite size scaling (FSS) [8,9], but may fail unless one manages to handle large system sizes (see below). Moreover, from a conceptual point of view, critical behavior manifests itself in the long wavelength limit. Real-space algorithms are, however, unable to take advantage of this fact.

In contrast, our newly developed Fourier Monte Carlo (FMC) algorithm [10] is tailor-made to deal with the problems listed above. In this algorithm, MC simulations are carried out exclusively in Fourier space, using the real an imaginary parts of the Fourier amplitudes $\tilde{s}(\boldsymbol{k})$ as MC variables. That such a type of simulation is feasible has recently been demonstrated by solving the long-standing problem of directly computing the gradient corrections to coarse-grained Landau-Ginzburg (LG) free energies derived from a lattice ϕ^4 Hamiltonian [10] from MC simulations. While we refer to Ref. [10] for a detailed description of this algorithm, here we only note that for the method to be applicable, it is necessary to rewrite the effective Hamiltonian purely in terms of the Fourier amplitudes $\tilde{s}(\boldsymbol{k})$, $\tilde{S}(\boldsymbol{k})$ of the spin field $s(\boldsymbol{x})$ and its accompanying squared spin configuration $S(\boldsymbol{x}) := s^2(\boldsymbol{x})$ in such a way that both amplitudes enter at most quadratically. Indeed, on a simple-cubic lattice of $L^3 = N$ sites with periodic boundary conditions and unit lattice constant, Eqn. (2) can be restated in the comparatively simple form

$$\mathcal{H}_{\text{eff}} = \sum_{\boldsymbol{k}} \left(\frac{Dk^2 + A_2}{2} |\tilde{s}(\boldsymbol{k})|^2 + \frac{A_4 - 2\tilde{\mathcal{K}}(\boldsymbol{k})}{4} |\tilde{S}(\boldsymbol{k})|^2 \right) \tag{4}$$

where $\tilde{\mathcal{K}}(\boldsymbol{0})$ is replaced by zero in the constant homogeneous strain ensemble, $\tilde{s}(\boldsymbol{k}) = N^{-(1/2)} \sum_{\boldsymbol{x}} s(\boldsymbol{x}) e^{-i\boldsymbol{k}\boldsymbol{x}}$, and $\tilde{S}(\boldsymbol{k}) = N^{-(1/2)} \sum_{\boldsymbol{p}} \tilde{s}(\boldsymbol{p}) \tilde{s}(\boldsymbol{k} - \boldsymbol{p})$. Moreover, we introduce the following novel modification of the finite size scaling approach. In studying critical behavior, we can drastically increase the accessible linear system size L by introducing a relatively small cubic cutoff $\Lambda(l) := 2\pi l/L$, $l \ll L/2$ in the discrete Brillouin zone (BZ), which represents a huge advantage over real-space based approaches. The effect of the residual modes with $\boldsymbol{k}$-vectors outside of this cutoff is absorbed in assuming a linear T-dependence $A_2(T) = A_0(T - T_0)$, while D and A_4 are kept T-independent, such that $\mathcal{H}_0$ actually resembles a universal coarse-grained LG Hamiltonian [10]. When using FSS on such an effective Hamiltonian with cutoff, only systems with equal fractions of vectors inside and outside the cutoff $\Lambda(l)$ in the BZ can be compared in a meaningful way. This requirement leads to a classification [10] of systems of size L and imposed cutoff $\Lambda(l)$ into families (L, l) with common label $\sigma(L, l) := L/(2l + 1)$. For the present simulations, we focused on the "small" cutoff ($\sigma = 4$) family $\{(12, 1), (20, 2), (28, 3), (36, 4), \ldots\}$.

For a general crystal class and a given set of bare elastic constants, $\tilde{\mathcal{K}}(\boldsymbol{k})$ can in principle be tabulated for all relevant $\boldsymbol{k}$-vectors during the startup of the simulation. Should there exist $\boldsymbol{k}$-vectors, for which $A_4 - 2\tilde{\mathcal{K}}(\boldsymbol{k}) < 0$, then stability would force one to add higher, e.g., sixth order terms $(A_6/6)s^6$, $A_6 > 0$, to the bare Hamiltonian. A standard mean field analysis then yields a trivial [2]" first-order phase transition (cf. Ref. [11]). In cubic systems, this is excluded if the stability condition

$$A_4 > 2g_0^2\kappa_0 \tag{5}$$

holds. In this more interesting case, a naive mean field treatment (for which the specific heat exponent α_0 of the rigid model is always zero) would therefore yield a second order transition. Nevertheless, for arbitrary cubic systems at constant pressure with $\alpha_0 > 0$ and anisotropic ones at constant volume, a refined RG analysis [2,7] predicts a fluctuation-induced first-order transition. According to Bergman and Halperin [7], a second order transition should only be expected for isotropic cubic systems under the quite restrictive assumption that not only the total volume in fixed but even each individual lattice site on the surface of the crystal is pinned. If $\alpha_0 > 0$, the exponents of this second order transition should be "Fisher-renormalized," i.e., $\alpha = -\frac{\alpha_0}{1-\alpha_0}$, $\beta = \frac{\beta_0}{1-\alpha_0}$, $\gamma = \frac{\gamma_0}{1-\alpha_0}$, $\nu = \frac{\nu_0}{1-\alpha_0}$. Theoretically, for periodic boundary conditions, first-order transitions should thus occur in all of the cases listed above. However, for extremely weak first-order transitions, where the correlation length remains finite but reaches values that are comparable to L, the actual crossover from a pseudocritical to first-order behavior may be hard or even impossible to resolve using FSS [12].

The present simulations were undertaken with the following common set of parameters: $D = 0.01$, $A_0 = 1.0$, $T_0 = 1.0$ in arbitrary units. At fixed compressibility $\kappa_0 = 1.3$, the bare cubic elastic constants C_{12}^0 and C_{44}^0 were parametrized by varying C_{11}^0 and the anisotropy parameter A' [7]. Finally, the common choice $g_0 = 0.55$ guarantees the stability condition of Eqn. (5). From the perspective of pure Landau theory, the constant homogeneous strain ensemble is certainly the most remote one. In the case of elastic isotropy ($A' = 0$), choosing $C_{11}^0 = 0.8$ and thus $C_{12}^0 = 0.7538$, $C_{44}^0 = 0.023$, the minima of the energy cumulant $E_4 = 1 - \langle E^4 \rangle / 3\langle E^2 \rangle^2$ are seen to rapidly approach the trivial value of $2/3$ with growing L, which signals a second order transition (cf. the insets of Fig. 1). At their common [13] intersection temperature $T_c = 0.588$, the intersection height $B_4^* := B_4^{(L,l)}(T_c) \approx 0.44$ of the so-called Binder cumulant $B_4 = 1 - \langle m^4 \rangle / 3\langle m^2 \rangle^2$ related to the magnetization per site $m = N^{-1} \sum_{\boldsymbol{x}} s(\boldsymbol{x})$ differs markedly from the universal Ising value $B_4^{*\text{Ising}} \approx 0.47$ (main part of Fig. 1). Following further standard procedures of FSS, an evaluation of the logarithmic T-derivatives of the observables B_4, $\langle |m| \rangle$, $\langle m^2 \rangle$, and $\langle m^4 \rangle$ at T_c yields a critical exponent $\nu = 0.7 \pm 0.04$, which, considering the value $\alpha_0^{\text{Ising}} = 0.108$ of the specific heat

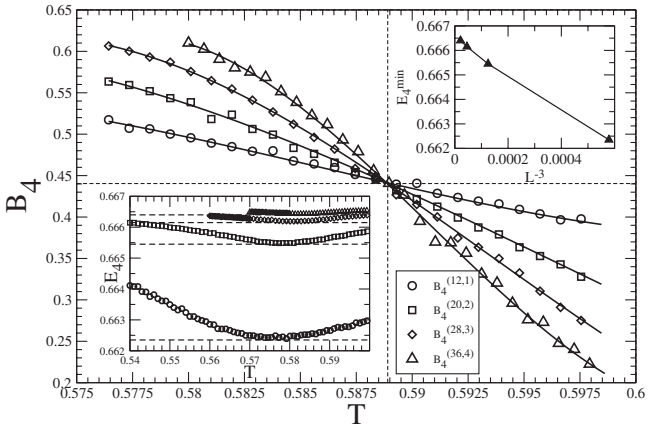

FIG. 1. Cumulants for $A' = 0$, $C_{11}^0 = 0.8$. Main figure: T-dependence of Binder cumulants $B_4^{(L,l)}(T)$ in the vicinity of common intersection temperature T_c. Left inset: T-dependence of energy cumulants $E_4^{(L,l)}(T)$. Right inset: scaling behavior of the minima of $E_4^{(L,l)}$ with inverse system volume L^{-3}.

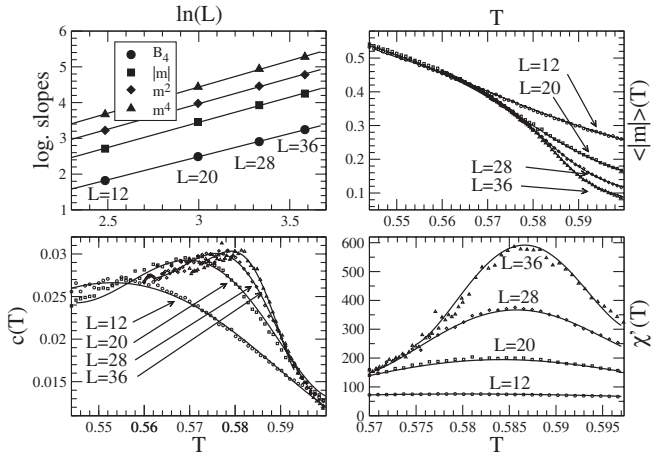

FIG. 2. Left upper plot: logarithmic slopes of B_4, $\langle m^2 \rangle$, and $\langle m^4 \rangle$ at T_c. Remaining plots: fits of MC data for $c(T)$, $\langle |m| \rangle (T)$, and $\chi'(T)$ over their common x-domain using Fisher-renormalized exponents combined with the FSS ansatz (6).

exponent for the pure $3d$ Ising model, is in excellent agreement with a Fisher-renormalized value $\nu = 0.705045$ of the $3d$ Ising exponent $\nu_0^{\text{Ising}} \approx 0.6289$. The peaks of the recorded specific heat data show a tendency to saturate rather than diverge with growing L, indicating a change of sign of α with respect to $\alpha_0 > 0$, which, apart from precision of numerical values, certainly represents the most striking fingerprint of Fisher renormalization [14] (cf. left upper plot of Fig. 2). For further confirmation, the MC observables $O = c(\tau)$ (specific heat), $\langle |m| \rangle (\tau)$ (modulus of magnetization), and $\chi' = N(\langle m^2 \rangle - \langle |m| \rangle^2)/k_B T$ (modified susceptibility [15]) were compared to the universal FSS ansatz [13,16]

$$\langle O \rangle = L^{\lambda_O/\nu}[f_O(x) + L^{-\omega} h_O(x) + \ldots], \qquad x := L^{1/\nu}\tau \tag{6}$$

where $\lambda_O \equiv \alpha, -\beta, \gamma$, respectively. Given the universal function $h_O(x)$, the rescaled data $L^{-\lambda/\nu}\langle O \rangle(\tau)$ should collapse onto the universal function $f_0(x)$ after subtraction of $L^{-\omega} h_O(x)$ when parametrized by x. Taylor expanding the subleading universal scaling correction functions $h_O(x)$ to fifth order and treating the expansion coefficients as fit parameters, this was indeed found to be possible using precisely the Fisher-renormalized exponents corresponding to their $3d$ Ising counterparts and a Wegner-correction exponent [16] $\omega \sim 0.8$ (cf. Figure 2). In summary, to the best of our knowledge, convincing evidence for Fisher renormalization of elastic systems is observed in simulations for the first time.

For $A' = 0$ and at fixed $\kappa_0 = 3/(C_{11}^0 + 2C_{12}^0) > 0$, we are still free to vary $C_{11}^0 > 0$ as long as the bare stability conditions $C_{44}^0 > 0$ and $C_{11}^0 > C_{12}^0$ are satisfied. If C_{11}^0 is chosen large enough at fixed bare compressibility κ_0, these conditions also allow for the somewhat unusual possibility $C_{12}^0 < 0$ which characterizes so-called *auxetic* materials which display an expansion in directions transverse to a certain uniaxial tensile loading. For $\kappa_0 = 1.3$ and $C_{11}^0 = 10.$, we get $C_{12}^0 = -3.846$ and $C_{44}^0 = 6.923$. For these parameter values, our simulations reveal clear signs of a first-order transition. As can be seen in Fig. 3, the Binder cumulants $B_4^{(L,l)}$ show negative branches, and the minima of the energy cumulants $E_4^{(L,l)}$ converge towards $E_4^{\infty} < 0.634$. In passing, we note that while these FSS findings stringently prove the first-order character of the bulk transition, typical first-order behavior was also found in additional Wang-Landau simulations of the order parameter probability distribution for a given finite (L, l)-system. With respect to variation of C_{12}^0, we are thus led to predict the existence of a tricritical point. In a first naive guess, neglecting corrections to the bare value resulting from the

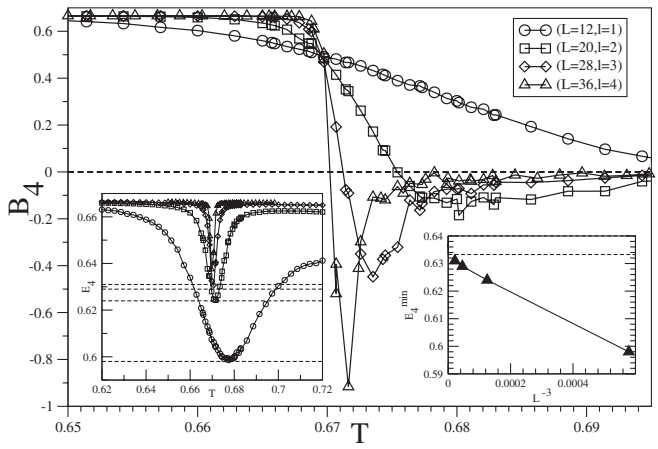

FIG. 3. Cumulants for $A' = 0$, $C_{11}^0 = 10.0$. Lines are a guide to the eye. Main figure: $B_4^{(L,l)}(T)$. Left inset: Temperature dependence of energy cumulants $E_4^{(L,l)}(T)$. Right inset: dependence of minima of $E_4^{(L,l)}$ on L^{-3}.

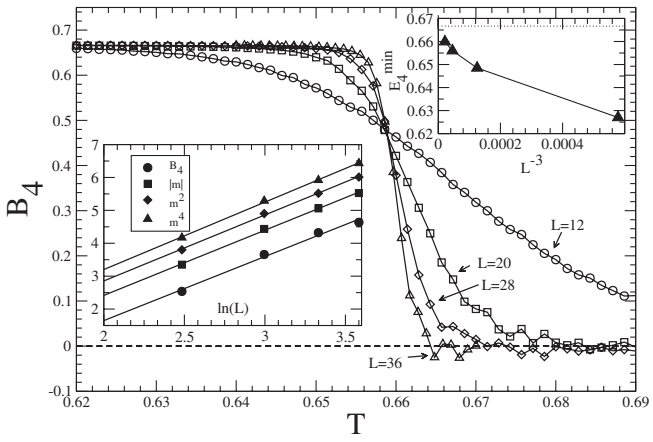

FIG. 4. Binder cumulants $B_4^{(L,l)}(T)$ for $A' = 0$, $C_{12}^0 = 0.0$. Left inset: logarithmic slopes of B_4, $\langle|m|\rangle$, $\langle m^2\rangle$, and $\langle m^4\rangle$ at T_c. Right inset: dependence of minima of $E_4^{(L,l)}$ on L^{-3}.

RG flow of C_{12}^0, we estimate its location at $C_{12}^0 = 0$, which results from choosing $C_{11}^0 = 2.307$. Indeed, at these parameter values, the Binder cumulants $B_4^{(L,l)}(T)$, which intersect at $B_4^* = B_4^{(L,l)}(T_c) \approx 0.475$, are found to fluctuate around zero in some temperature region above $T_c = 0.6588$ (cf. Figure 4), and the minima of the energy cumulants $E_4^{(L,l)}$ seem to slowly converge towards $2/3$. A calculation of the exponent ν by FSS yields $\nu = 0.5 \pm 0.02$ reminiscent of a weak first-order transition [16] (cf. inset of Fig. 4).

For nonauxetic but elastically anisotropic systems, we are currently unable to explicitly verify the first-order character predicted by theory. In fact, the FSS observed is similar to criticality, but the computed exponents appear to be nonuniversal. For instance, for C_{11}^0 and $A' = 0.9$, we find $\nu = 0.6734 \pm 0.03$, whereas at $A' = 1.0$, we have $\nu = 0.76 \pm 0.05$. We interpret the appearance of these nonuniversal exponents as pseudocritical behavior, i.e., a crossover precursor to another critical RG fixed point or a possibly weak first-order transition that may be clearly detectable only for system sizes exceeding those accessible to the present simulations. Of course, this may also be the case for isotropic systems, where we observed the Fisher-renormalized exponents and argued about the possibility of a tricritical point. In comparing theoretical predictions to our results, one must be aware that the boundary condition of fixed homogeneous strain is somewhat less restrictive than Bergman and Halperin's condition of pinned surface atoms, which also excludes the appearance of surface waves, but stricter than that of mere constant total volume. Passing to the constant stress ensemble, we report the observation of first-order transitions for all considered parameters in the FSS analysis. The corresponding behavior of cumulants is quite similar to that shown in Fig. 3. Because of space limitations, further details are omitted here. Our approach is generalizable to n-vector models with anisotropic fourth order couplings on noncubic lattices and, e.g., bilinear order parameter-strain couplings.

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