Universal Effective Potential for Scalar Field Theory in Three Dimensions by Monte Carlo Computation

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We study the low-energy effective action for the theory of a one-component real scalar field in three Euclidean dimensions (3D), in the symmetric phase, concentrating on its static part—effective potential $V_{\mathrm{eff}}(\varphi)$. We compute it from the probability distributions of the average magnetization in the 3D Ising model in an external field, obtained by Monte Carlo computation. We find that the φ^6 term in V_{eff} is important in 3D, and compute the values of the universal four-point and six-point couplings.

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This work is devoted to the following problem: What is the effective potential, and the corresponding effective Ginzburg-Landau theory, that would provide not an exact, but a reasonably phenomenologically accurate description of the properties of the 3D Ising model (and other models in the same universality class) near the phase transition?

The model in this universality class that is particularly suitable for field-theoretical treatment is the theory of one-component real scalar field in three Euclidean dimensions ("3D ϕ^4 theory"), defined by the (bare) action

$$S = \int d^3x \left\{ \frac{1}{2}\partial_\mu\phi\partial_\mu\phi + \frac{1}{2}m^2\phi^2 + \lambda\phi^4 \right\}. \quad (1)$$

Thus, from the field-theoretical point of view, we study the low-energy effective action of this theory.

This problem, being interesting by itself (it is closely related to the Ising equation of state), is also relevant to the theory of cosmological phase transitions in the early Universe. The second-order high-temperature phase transition in the (3 + 1)-dimensional quantum field theory is in the universality class of the 3D Euclidean phase transition. Weak first-order high-temperature transitions can be studied in the framework of effective 3D Euclidean theory as well. The effective potential for such problems has been a subject of recent investigations [1]. The use of the perturbation theory is hindered in three dimensions by infrared divergences and by the strong-coupling nature of the problem, and leads to controversy over such points as existence and the role of the $|\varphi|^3$ term in the effective potential.

Thus, the nonperturbative study of the effective action of the simplest 3D field theory (1), or that of the 3D Ising model, seems appropriate.

The model.—We study the Ising model with the nearest-neighbor interaction on a simple cubic lattice. The partition function is

$$Z = \sum_{\{\phi_i\}} \exp\left\{ \beta\sum_{\langle ij\rangle}\phi_i\phi_j + J\sum_i\phi_i \right\}, \quad \phi_i = \pm 1, \quad (2)$$

where J is the homogeneous external field. We study the symmetric (paramagnetic) phase, the coupling β being less than, but close to, the critical value $\beta_c \approx 0.221\,65$.

Our main subjects are the long-wave (low-momentum, low-energy) properties of the model, when it is in the scaling region, but not exactly at the critical point. Then the properties are fixed, and the only free parameter is the mass (= scale). The particles of the corresponding (2 + 1)-dimensional field theory are massive (and thus can be nonrelativistic) and have well-defined low-energy properties, such as nonrelativistic scattering amplitudes. The effective action we are looking for is a convenient formalism to describe these properties.

The effective action.—The low-energy Ginzburg-Landau-Wilson effective action can be written as

$$S_{\mathrm{eff}} = \int d^3x \left\{ \frac{1}{2}Z_\varphi^{-1}\partial_\mu\varphi\partial_\mu\varphi + V_{\mathrm{eff}}(\varphi) - J(x)\varphi(x) \right\},$$
$$V_{\mathrm{eff}} = r\varphi^2 + (\text{higher terms}), \quad (3)$$

where $\varphi(x)$ is the (slowly varying) average magnetization, and we keep only the lowest-order gradient term. To compute S_{eff} one needs to know the effective potential $V_{\mathrm{eff}}(\varphi)$ and the field renormalization factor Z_φ. To compute the former, it is sufficient to consider only the homogeneous external field $J(x) = J$; the latter can be derived from the two-point correlation function of φ at $J = 0$.

Computation of V_{eff}.—For the computation of V_{eff} we have developed a method that is close in spirit to the constrained effective potential approach [2], but contains two significant improvements.

Thus, we derive V_{eff} from the probability distribution $P(\varphi)$ of the order parameter (magnetization per site, $\varphi = \frac{1}{N}\sum_i \phi_i$, where N is the total number of sites on the lattice) [3] in the finite volume system (Fig. 1). The first improvement is that we consider the distributions at several different values of J, and not only at $J = 0$. This makes it possible to study V_{eff} at larger values of φ, where the higher terms in V_{eff} become significant (the distribution at $J = 0$ is determined mostly by the quadratic term).

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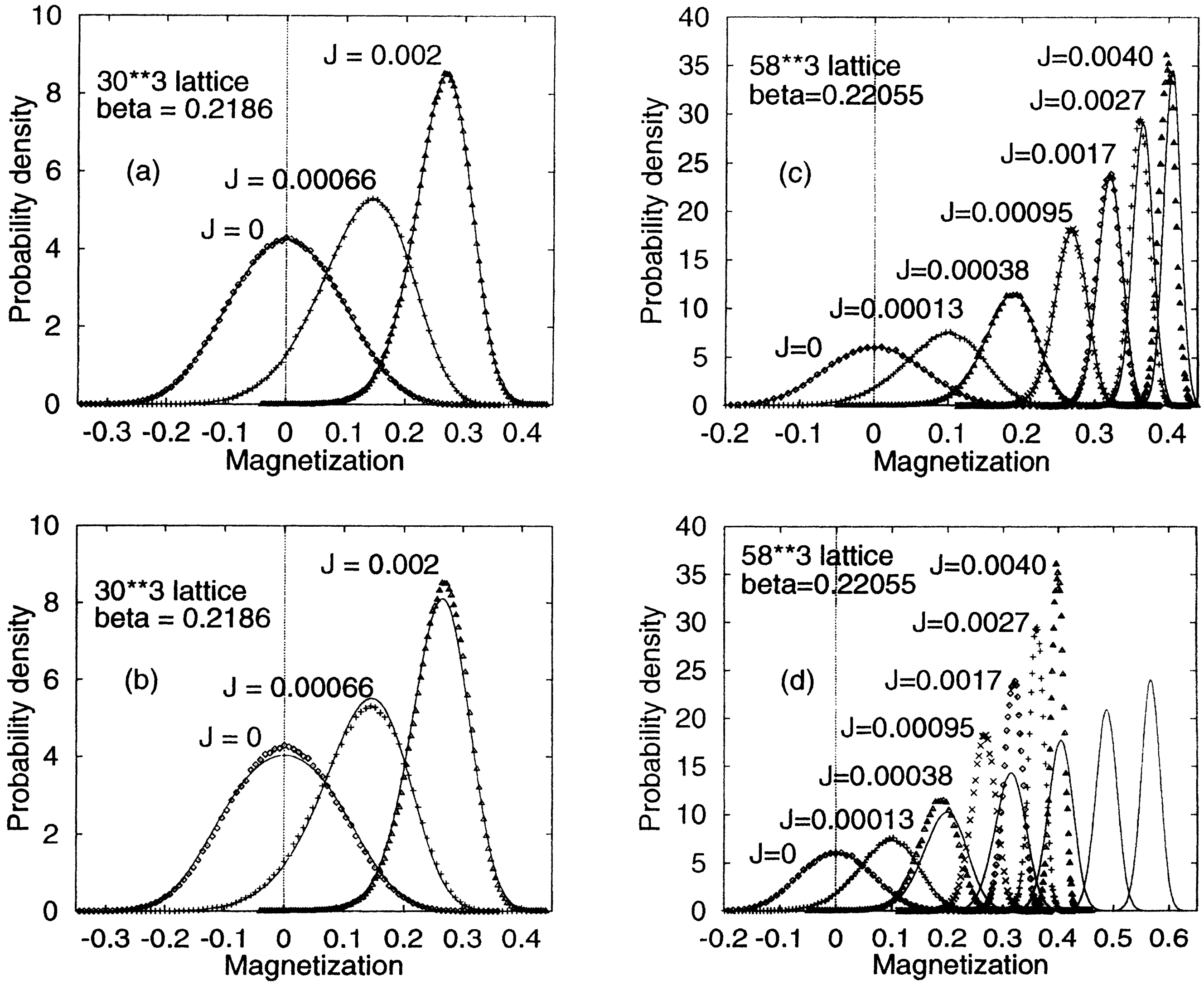

FIG. 1. The probability density $P(\varphi)$ for the magnetization per lattice site φ, for the Ising model (2). The solid line corresponds to (4), with $V_{\rm eff}$ chosen as follows: (a) $V_{\rm eff}(\varphi) = r\varphi^2 + u\varphi^4 + w\varphi^6$, three histograms fitted simultaneously; (b) the same for $V_{\rm eff}(\varphi) = r\varphi^2 + u\varphi^4$; (c) $V_{\rm eff}(\varphi) = r\varphi^2 + u\varphi^4 + w\varphi^6$, histograms for $J = 0$, 0.000 13, and 0.000 38 fitted simultaneously; (d) $V_{\rm eff}(\varphi) = r\varphi^2 + u\varphi^4$ with r and u taken from (c).

The second improvement is that we use the relation between $V_{\rm eff}(\varphi)$ and $P(\varphi)$ that takes into account the pre-exponential factor:

$$P(\varphi) \propto \left(\frac{d^2 V_{\rm eff}(\varphi)}{d\varphi^2}\right)^{1/2} \exp\{-\Omega V_{\rm eff}(\varphi) + \Omega J\varphi\}. \quad (4)$$

This is an asymptotic expression for a system in a finite box of volume Ω with periodic boundary conditions, for $\Omega \to \infty$. Practically, we see no deviation from it already for $L/\xi \gtrsim 4$, where ξ is the correlation length and the lattice size is L^3. This relation can be found, in various disguises, in the literature [4]. It seems to be useful for the theory of the order parameter probability distribution in general. For example, the statement that for the asymmetrical first-order transitions the two peaks of this distribution have equal weight rather than equal height at the transition point [5] is an immediate consequence of (4).

Monte Carlo computation.—We study the 3D Ising model (2) on a simple cubic lattice with periodic boundary conditions, on lattices from 14^3 to 58^3. The Swendsen-Wang cluster Monte Carlo algorithm in the external magnetic field [6] is used to generate the Boltzmann ensemble of configurations. (We use the version of this algorithm without the ghost spin.) For every configuration we measure magnetization per site $\varphi = \frac{1}{N}\sum_i \phi_i$ and compute the histograms for the probability density $P(\varphi)$, for several values of J. Then we do the simultaneous fit of several histograms with (4). (We minimize the sum of χ^2 from the individual histograms.) The first ansatz to try is

$$V_{\rm eff}(\varphi) = r\varphi^2 + u\varphi^4, \qquad (5)$$

inspired by the standard Ginzburg-Landau theory (or the tree-level ϕ^4 theory), where r and u are treated as fit parameters. However, as can be seen from Figs. 1(b) and 1(d), a good description of data with (5) cannot be achieved. When the histograms are fitted simultaneously [Fig. 1(b)], considerable discrepancy shows up in all of them. When the parameters r and u are chosen to describe correctly the properties at small φ [Fig. 1(d)], a discrepancy shows up at larger φ, indicating the presence of higher terms in $V_{\rm eff}$.

So we consider a three-parameter expression

$$V_{\rm eff}(\varphi) = r\varphi^2 + u\varphi^4 + w\varphi^6. \qquad (6)$$

We have found that it works very well, providing the ideal fit at Fig. 1(a) (no systematic discrepancy between data and fit, just noise), and only a small discrepancy shows up for the larger values of φ at Fig. 1(c). We have found no other reasonable ansatz that works so well.

Thus for every value of the bare coupling β we obtain the low-energy effective Lagrangian

$$\mathcal{L}_{\rm eff} = \frac{1}{2} Z_\varphi^{-1} \partial_\mu\varphi\partial_\mu\varphi + r\varphi^2 + u\varphi^4 + w\varphi^6. \qquad (7)$$

The three parameters r, u, and w are determined by the fitting procedure described above. The field renormalization factor Z_φ is obtained from the propagator in the momentum space

$$G_2(\mathbf{p}) = \langle\phi(\mathbf{p})\phi^*(\mathbf{p})\rangle, \quad \phi(\mathbf{p}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{x}} \phi_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}}, \qquad (8)$$

which behaves at small momentum p as

$$G_2(\mathbf{p})^{-1} = Z_\varphi^{-1} p^2 + 2r. \qquad (9)$$

After the renormalization of φ,

$$\varphi = \sqrt{Z_\varphi}\varphi_R, \qquad (10)$$

we obtain the effective Lagrangian in the form

$$\mathcal{L}_{\rm eff} = \frac{1}{2}\partial_\mu\varphi_R\partial_\mu\varphi_R + \frac{1}{2}m^2\varphi_R^2 + mg_4\varphi_R^4 + g_6\varphi_R^6, \qquad (11)$$

where

$$m = \sqrt{2Z_\varphi r}, \quad g_4 = \frac{Z_\varphi^2 u}{\sqrt{2Z_\varphi r}}, \quad g_6 = Z_\varphi^3 w. \qquad (12)$$

In the continuum limit ($m = \xi^{-1} \to 0$) this effective Lagrangian should be universal. Thus, the only free parameter is m, which determines the scale, while the dimensionless four- and six-point couplings g_4 and g_6 take definite values that are the same for the whole 3D Ising universality class.

Extrapolation to the continuum limit.—Apart from statistical errors, there are two sources of systematic errors: finite volume and finite ultraviolet cutoff. To check for the finite volume effects, we increase the lattice size L, keeping m fixed. We found that for $L/\xi \gtrsim 4$ finite volume effects are negligible. To check for the effect of the finite cutoff, we keep L/ξ fixed at ≈ 4.1, increase ξ, and scale J according to

$$J \propto \xi^{-\beta\delta/\nu} \quad (\beta\delta \approx 1.57,\ \nu \approx 0.63). \qquad (13)$$

It turns out that while for g_4 this effect is negligible at $\xi \gtrsim 4$, a considerable dependence of g_6 on ξ makes it necessary to extrapolate the data to $\xi \to \infty$ (Fig. 2). The reasonable extrapolation is $g_6(\xi) = g_6(\infty) + a\xi^{-\kappa}$. To get a reliable estimate of the exponent κ, we have considered the ξ dependence of such a linear combination of g_4 and g_6 that has the smallest statistical error, and found $\kappa = 1.5 \pm 0.2$. That is why we plot g_4 and g_6 as functions of $L^{-1.5}$. We obtain in the continuum limit

$$g_4 = 0.97 \pm 0.02, \quad g_6 = 2.05 \pm 0.15, \qquad (14)$$

where the errors are the standard deviations. The value of g_4 is in good agreement with the available data [7–10], providing a consistency check of our computation.

Some information on g_6 is also available in the literature, but much less than on g_4. The only Monte Carlo study we are aware of was performed by Wheater [10]. However, large statistical errors made it impossible to reach a definite conclusion about the value of g_6 in the continuum limit and whether it is different from zero.

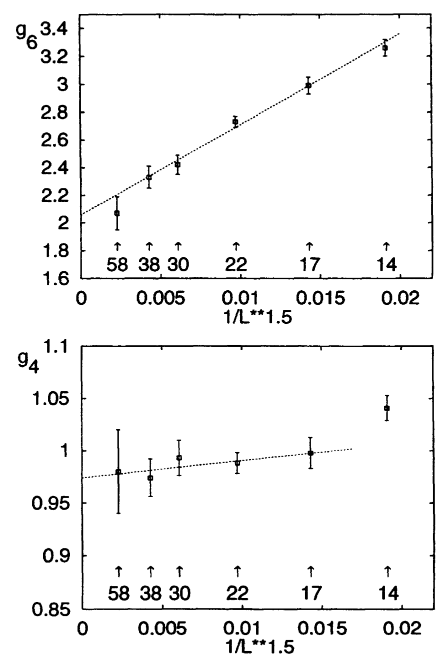

FIG. 2. The dimensionless four-point coupling g_4 and six-point coupling g_6 as functions of the lattice size L. The ratio L/ξ is kept at about 4.1. The errors shown are standard deviations.

The ϵ expansion for the Ising equation of state [11] leads to the relation

$$\frac{g_6}{(g_4)^2} = 2\epsilon - \frac{20}{27}\epsilon^2 + 1.2759\epsilon^3 + O(\epsilon^4), \qquad (15)$$

for the dimension of space $d = 4 - \epsilon$. Our result (14) is in reasonable agreement with this, as well as with the Wegner-Houghton equation [12] fixed point value $g_6^* = 2.40$ and "effective average action" computations [13] (fixed point value $g_6^* = 1.82$, low-energy coupling $g_6 = 2.23$).

However, our result disagrees with the strong-coupling expansion [14], which favors $g_6 = 0$, and with dimensional expansion [15], which favors $g_6 = \infty$.

Discussion.—A widespread point of view on the effective potential in 3D is as follows. The problem should be considered in the framework of the ϕ^4 theory. Then either one works on the tree level, and has the standard Landau theory (5), or one includes loop corrections, and then all powers of φ must be retained in $V_{\rm eff}$, φ^6 being treated on equal footing with other higher terms.

Our study corroborates an alternative point of view advocated by Tetradis and Wetterich [13] that, while (5) is a rather rough approximation, the ansatz (6) gives a very good approximation, for φ not too large, and the higher powers of φ can be considered as small corrections. This is related to the smallness of the critical index η in the 3D theory. Similar behavior is observed at the weak first-order transition in the 3D three-state Potts model [16].

This, together with the computation of the universal dimensionless coupling g_6, is our main result. As a by-product, we have checked the accuracy of the formula (4), which is of interest for the theory of the order parameter probability distribution.

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[1] K. Kajantie, K. Rummukainen, and M. Shaposhnikov, Nucl. Phys. **B407**, 356 (1993); M. Shaposhnikov, Phys. Lett. B **316**, 112 (1993).
[2] J. Goldstone, Nuovo Cimento **19**, 154 (1961); R. Fukuda and E. Kyriakopoulos, Nucl. Phys. **B85**, 354 (1975); P. Ginsparg and H. Levine, Phys. Lett. **131B**, 127 (1983); L. O'Raifeartaigh, A. Wipf, and H. Yoneyama, Nucl. Phys. **B271**, 653 (1986).
[3] K. Binder, Z. Phys. B **43**, 119 (1981).
[4] E. Brézin and J. Zinn-Justin, Nucl. Phys. **B257 [FS14]**, 867 (1985); V. Privman, in *Finite Size Scaling and Numerical Simulation of Statistical Systems,* edited by V. Privman (World Scientific, Singapore, 1990), p. 1; see Sect. 5.6.3; M. Göckeler and H. Leutwyler, Nucl. Phys. **B350**, 228 (1991).
[5] K. Binder and D.P. Landau, Phys. Rev. B **30**, 1477 (1984); C. Borgs and R. Kotecký, J. Stat. Phys. **61**, 79 (1990); Phys. Rev. Lett. **68**, 1734 (1992); V. Privman and J. Rudnick, J. Stat. Phys. **60**, 551 (1990).
[6] R.H. Swendsen and J.-S. Wang, Phys. Rev. Lett. **58**, 86 (1987); J.-S. Wang and R.H. Swendsen, Physica (Amsterdam) **167A**, 565 (1990); J.-S. Wang, *ibid.*, **161A**, 249 (1989).
[7] G.A. Baker *et al.,* Phys. Rev. Lett. **36**, 1351 (1976); Phys. Rev. B **17**, 1365 (1978); J.C. Le Guillou and J. Zinn-Justin, Phys. Rev. Lett. **39**, 95 (1977); Phys. Rev. B **21**, 3976 (1980); B.G. Nickel, Physica (Amsterdam) **177A**, 189 (1991).
[8] G.A. Baker and J.M. Kincaid, Phys. Rev. Lett. **42**, 1431 (1979); J. Stat. Phys. **24**, 469 (1981).
[9] B. Freedman, P. Smolensky, and D. Weingarten, Phys. Lett. **113B**, 481 (1982); B.A. Freedman and G.A. Baker, J. Phys. A **15**, L715 (1982); R.A. Weston, Phys. Lett. B **219**, 315 (1989); J.-K. Kim and A. Patrascioiu, Phys. Rev. D **47**, 2588 (1993).
[10] J.F. Wheater, Phys. Lett. **136B**, 402 (1984).
[11] G.M. Avdeeva and A.A. Migdal, JETP Lett. **16**, 178 (1972); E. Brézin, D.J. Wallace, and K.G. Wilson, Phys. Rev. Lett. **29**, 591 (1972); D.J. Wallace and R.K.P. Zia, J. Phys. C **7**, 3480 (1974); D.J. Wallace, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M.S. Green (Academic Press, London, 1976), Vol. 6, p. 293; J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Clarendon Press, Oxford, 1989); see Sect. 25.1.3.
[12] C. Bagnuls and C. Bervillier, Phys. Rev. B **41**, 402 (1990).
[13] M. Reuter, N. Tetradis, and C. Wetterich, Nucl. Phys. **B401**, 567 (1993); N. Tetradis and C. Wetterich, DESY Report No. 93-094 (1993); DESY Report No. 93-128 (1994); N. Tetradis (private communication).
[14] C.M. Bender *et al.,* Phys. Rev. Lett. **45**, 501 (1980); Phys. Rev. D **23**, 2976 (1981); Phys. Rev. D **23**, 2999 (1981).
[15] C.M. Bender and S. Boettcher, Phys. Rev. D **48**, 4919 (1993).
[16] M.A. Stephanov and M.M. Tsypin, Nucl. Phys. **B366**, 420 (1991).