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RENORMALIZATION-GROUP THEORY OF CRITICAL PHENOMENA IN CONFINED SYSTEMS: ORDER-PARAMETER DISTRIBUTION FUNCTION

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We present a renormalization-group study of the order-parameter distribution function near the critical point of O(n) symmetric three-dimensional (3D) systems in a finite geometry. The distribution function is calculated within the φ^4 field theory for a 3D cube with periodic boundary conditions by means of a novel approach that appropriately deals with the Goldstone modes below T_c. Results are given for both vanishing and finite external field h. The results describe finite-size effects near the critical point in the h–T-plane including the first-order transition at the coexistence line at $h = 0$ below T_c. Quantitative theoretical predictions of the finite-size scaling function are presented for the Ising ($n = 1$), XY ($n = 2$) and Heisenberg ($n = 3$) models. Good agreement is found with recent Monte Carlo data.

1. Introduction

The interest in finite-size effects on phase transitions has remained on a highly stimulating level over the last years. Perhaps the most fundamental quantity in the statistical description of these effects is the probability distribution $P(\mathbf{\Phi})$ of the spatial average $\mathbf{\Phi}$ of the order-parameter,[1]

$$\mathbf{\Phi} = V^{-1} \int d^d x \varphi(x) , \tag{1}$$

where $\varphi(x)$ represents the local fluctuating order-parameter variable in a continuum description with V being the finite volume. $P(\mathbf{\Phi})$ determines the finite-size effects on various important thermodynamic quantities such as the susceptibility, specific heat and the order parameter (equation of state). This distribution function can be studied both for Ising-like systems as well as for O(n) symmetric systems such as XY-like ($n = 2$) and Heisenberg-like ($n = 3$) systems where $\mathbf{\Phi}$ is an n component vector. Performing these studies at finite external field $\mathbf{h}$ includes both the finite-size critical behavior in the h-T plane near $T = T_c$ as well as the finite-size effects at the first-order transition at $T < T_c$ as $\mathbf{h}$ changes sign. These effects are of particular interest in O(n) symmetric systems with $n \geq 2$ where the massless spin-wave (Goldstone) modes govern the long-distance properties for $\mathbf{h} \to 0$ below T_c.

So far no theoretical predictions of $P(\mathbf{\Phi})$ are available for $O(n)$ symmetric systems below T_c that include both first-order and critical finite-size effects as a function of $\mathbf{h}$ for $T \approx T_c$. In this paper we present a field-theoretic study of $P(\mathbf{\Phi})$ of the $O(n)$ symmetric φ^4 model in a three-dimensional (3D) cube with periodic boundary conditions both for $\mathbf{h} = 0$ and for $\mathbf{h} \neq 0$. In order to cope with the notorious difficulty in treating the Goldstone modes near T_c we shall use a novel approach[2,3] that satisfactorily deals with the Goldstone problems in a *nonperturbative* way. Quantitative predictions are presented for the finite 3D Ising-, XY- and Heisenberg-models and good agreement with recent Monte Carlo (MC) data above, at and below T_c is found.

2. Bare Theory

Our treatment is based on the φ^4 model with the standard Landau–Ginzburg–Wilson Hamiltonian

$$H(\mathbf{h}) = \int_V d^d x \left[\frac{1}{2} r_0 \varphi^2 + \frac{1}{2} (\nabla\varphi)^2 + u_0 \varphi^4 - \mathbf{h}\cdot\varphi\right] \tag{2}$$

where $\varphi(x) = L^{-d}\sum_k \varphi_k e^{ikx}$ is an n-component field in a finite cube of volume $V = L^d$ with periodic boundary conditions and $\mathbf{h}$ is a homogeneous external field. The summation $\sum_k$ runs over discrete $\mathbf{k}$ vectors with components $k_j = 2\pi m_j/L$, $m_j = 0, \pm1, \pm2, \ldots, j = 1, 2, \ldots, d$ in the range $|k_j| \leq \Lambda$. The temperature enters through $r_0 = r_{0c} + a_0 t$, $t = (T - T_c)/T_c$. Pioneering work on finite-size calculations within this model has been performed previously[4,5] for $T \geq T_c$ at $\mathbf{h} = 0$ where it was proposed to decompose $\varphi(x)$ as

$$\varphi(x) = \mathbf{\Phi} + \sigma(x) \tag{3}$$

and to treat the inhomogeneous modes

$$\boldsymbol{\sigma}(x) = L^{-d} \sum_{k\neq 0} \varphi_k \, e^{ikx} \tag{4}$$

perturbatively while the lowest mode $\mathbf{\Phi}$, Eq. (1), was treated exactly. These calculations, however, did not yet provide an appropriate concept for the case $T < T_c$. Recently such a concept was developed for $n = 1$[6] which, however, turned out not to be extendable to the case $n \geq 1$.[7] Here we present a novel concept that is appropriate for general n both at $\mathbf{h} = 0$[2] and $\mathbf{h} \neq 0$.[3]

The order-parameter distribution function $P(\mathbf{\Phi}) \equiv P(\mathbf{\Phi}, t, \mathbf{h}, L)$ is defined by functional integration over σ,

$$P(\mathbf{\Phi}, t, \mathbf{h}, L) = Z(\mathbf{h})^{-1} \int D\sigma e^{-H(\mathbf{h})}\,, \tag{5}$$

where

$$Z(\mathbf{h}) = \int d^n\mathbf{\Phi} \int D\sigma e^{-H(\mathbf{h})}\,. \tag{6}$$

Substituting the decomposition of φ, Eq. (3), into Eq. (2) yields

$$H(\mathbf{h}) = H_0(\mathbf{\Phi}, \mathbf{h}) + H'(\mathbf{\Phi}, \sigma)\,, \tag{7}$$

$$H_0(\mathbf{\Phi}, \mathbf{h}) = L^d \left(\frac{1}{2} r_0 \Phi^2 + u_0 \Phi^4 - \mathbf{h} \cdot \mathbf{\Phi}\right)\,, \tag{8}$$

$$H'(\mathbf{\Phi}, \sigma) = \int_V d^d x \left\{ \frac{1}{2} [r_{0L} \sigma_L^2 + r_{0T} \sigma_{0T}^2 + (\nabla \sigma_L)^2 + (\nabla \sigma_T)^2] + 4 u_0 \mathbf{\Phi} \sigma_L \sigma^2 + u_0 \sigma^4 \right\} \tag{9}$$

with the longitudinal and transverse parameters $r_{0L} = r_0 + 12 u_0 \Phi^2$, $r_{0T} = r_0 + 4 u_0 \Phi^2$. Here we have further decomposed $\sigma = \sigma_L + \sigma_T$ into longitudinal and transverse parts that are parallel and perpendicular to the vector $\mathbf{\Phi}$, respectively, with $\sigma^2 = \sigma_L^2 + \sigma_T^2$. This yields the distribution function in the form

$$P(\mathbf{\Phi}) = (Z^{\text{eff}})^{-1} e^{-H^{\text{eff}}(\mathbf{\Phi})}\,, \tag{10}$$

$$H^{\text{eff}}(\mathbf{\Phi}) = H_0(\mathbf{\Phi}, \mathbf{h}) + \Gamma(\Phi) - \Gamma(0)\,, \tag{11}$$

$$\Gamma(\Phi) = -\ln \int D\sigma_L D\sigma_T e^{-H'}\,, \tag{12}$$

with $Z^{\text{eff}} = \int d^n \mathbf{\Phi} \exp[-H^{\text{eff}}]$. In Eq. (11) the constant $\Gamma(0)$ has been subtracted for convenience. This permits to let $\Lambda \to \infty$ in the renormalized theory without generating *additive* ultraviolet divergencies of $H^{\text{eff}}(\mathbf{\Phi})$. Note that at this stage of the theory the $\mathbf{h}$ dependence enters only through $H_0(\mathbf{\Phi}, \mathbf{h})$.

The main problem is to develop a perturbation approach to calculate $\Gamma(\Phi)$, Eq. (12). Thus the basic question arises how to split

$$H'(\mathbf{\Phi}, \sigma) = H_1 + H_2 \tag{13}$$

into an unperturbed part H_1 and a perturbation part H_2. The Gaussian parts of H', Eq. (9), are obviously problematic for $r_0 < 0$ and cannot be used as H_1 because both r_{0L} and r_{0T} become negative for small Φ^2 and k^2. This problem has been solved perturbatively for $n = 1$ and $\mathbf{h} = 0$[6] by replacing $\Phi^2 \to M_0^2$ in the longitudinal Gaussian part of H_1 where

$$M_0^2 = Z_0^{-1} \int d^n \mathbf{\Phi} \Phi^2 e^{-H_0(\mathbf{\Phi}, 0)} \tag{14}$$

with

$$Z_0 = \int d^n \mathbf{\Phi} e^{-H_0(\mathbf{\Phi}, 0)}\,. \tag{15}$$

Clearly this works also for $\mathbf{h} \neq 0$ with $M_0^2(h)$ determined by $H_0(\mathbf{\Phi}, \mathbf{h})$, Eq. (8). This is not applicable, however, to the transverse part. Although the transverse parameter $\tilde{r}_{0T} = r_0 + 4u_0 M_0^2(h)$ remains positive for $r_0 \leq 0$ as long as L or $\mathbf{h}$ are finite, it becomes a dangerous parameter in the limit $L \to \infty$, $\mathbf{h} \to 0$ or $\mathbf{h} \to 0$, $L \to \infty$ where $\tilde{r}_{0T}$ vanishes for $r_0 \leq 0$ since M_0^2 approaches the mean-field value $-r_0/4u_0$. This would cause (spurious) Goldstone singularities in a conventional perturbation approach[7] for $L \to \infty$, $\mathbf{h} \to 0$ or $\mathbf{h} \to 0$, $L \to \infty$ and would yield unreliable perturbative results for $\Gamma(\Phi)$ at sufficiently small h and large L.

In the following we present a solution to this problem. A simple but important observation is the fact that the distribution function $e^{-H'}$ determining $\Gamma(\Phi)$ is well behaved for large σ not only for $r_0 \geq 0$ but also for $r_0 < 0$ owing to the positivity of the last term $H^{(4)} = \int d^dx\, u_0 \sigma^4$ in Eq. (9). Consider $H^{(4)}$ in terms of the Fourier amplitudes $\varphi_k \equiv \sigma_k = \sigma_{Lk} + \sigma_{Tk}$ with $\sigma_0 \equiv 0$,

$$H^{(4)} = u_0 L^{-3d} \sum_{kk'k''} (\sigma_k \sigma_{k'})(\sigma_{k''} \sigma_{-k-k'-k''}) \,. \tag{16}$$

The basic idea of our new approach is to include a *tractable* part of this positive term in H_1 such that e^{-H_1} remains well behaved for large σ even for $r_0 < 0$. In constructing H_1 we have been guided by the idea of generalizing the non-perturbative treatment of the $k = 0$ Hamiltonian H_0, Eq. (8), to finite $\mathbf{k}$. We shall show that this is achieved by defining

$$H_1 = \sum_k [H_k^{(2)} + H_k^{(4)}] \,, \tag{17}$$

$$H_k^{(2)} = \frac{1}{2} L^{-d} [(r_{0L} + k^2)|\sigma_{Lk}|^2 + (r_{0T} + k^2)|\sigma_{Tk}|^2] \,, \tag{18}$$

$$H_k^{(4)} = 3u_0 L^{-3d} [|\sigma_{Lk}|^4 + |\sigma_{Tk}|^4] \,, \tag{19}$$

where $H_k^{(4)}$ originates from $H^{(4)}$ for the special cases $\mathbf{k}' = -\mathbf{k}$, $\mathbf{k}'' = \mathbf{k}$ or $\mathbf{k}' = -\mathbf{k}$, $\mathbf{k}'' = -\mathbf{k}$ or $\mathbf{k}' = \mathbf{k}$, $\mathbf{k}'' = -\mathbf{k}$; the factor of 3 in Eq. (19) takes into account the number of possibilities to combine the Fourier amplitudes of Eq. (16) in factors of the form $|\sigma_{Lk}|^4$ and $|\sigma_{Tk}|^4$.

We emphasize that, unlike $H^{(4)}$, the last term of H_1 is a *single* sum that will not contribute to bulk quantities because of the prefactor L^{-3d} of $H_k^{(4)}$. This implies that the coupling of the last term of H_1 is $u_0 L^{-2d}$ rather than u_0. It is only the first term of H_1 that yields the usual one-loop bulk contribution to the free energy. Nevertheless, for finite L and $r_0 < 0$, $H_k^{(4)}$ plays the role of a regulator that is crucial, both for $\mathbf{h} = 0$ and $\mathbf{h} \neq 0$, in order to ensure the positivity of the small-k part of H_1 in the region $r_{0L} + k^2 < 0$ and $r_{0T} + k^2 < 0$.

In the following we shall neglect H_2 of Eq. (13). As far as bulk contributions are concerned this corresponds to a one-loop approximation. Then we obtain

$$\Gamma(\Phi) = -\ln \int \prod_{k\neq 0} d\sigma_{Lk} d\sigma_{Tk} \exp\left(- H_k^{(2)} - H_k^{(4)} \right) . \tag{20}$$

We see that the particular choice of the fourth-order term in Eq. (19) is crucial for the tractability of the non-Gaussian functional integral which is split up into *uncoupled* integrations for each $\mathbf{k} = 2\pi\mathbf{m}/L$. This permits to treat $H_k^{(4)}$ *non-perturbatively* and leads to the (bare) effective Hamiltonian

$$H^{\text{eff}}(\mathbf{\Phi}) = H_0(\mathbf{\Phi}, \mathbf{h}) - \frac{1}{2} \sum_{\mathbf{m}\neq 0} \ln \left\{ \frac{Z_1[y_{0\mathbf{m}}(r_{0L})]}{Z_1[y_{0\mathbf{m}}(r_0)]} \right\}$$

$$- \frac{1}{2}(n-1) \sum_{\mathbf{m}\neq 0} \ln \left\{ \frac{Z_1[y_{0\mathbf{m}}(r_{0T})]}{Z_1[y_{0\mathbf{m}}(r_0)]} \right\} , \tag{21}$$

$$y_{0\mathbf{m}}(r) = \left(\frac{2L^{d-4}}{3u_0} \right)^{1/2} (rL^2 + 4\pi^2\mathbf{m}^2) , \tag{22}$$

$$Z_1[y] = \int_0^\infty ds \; s \exp\left(-\frac{1}{2} y s^2 - s^4 \right) . \tag{23}$$

This Hamiltonian is the analytic basis of this paper. It is applicable for $r_0 \geq 0$ and $r_0 < 0$ and is free of Goldstone singularities in the limit $L \to \infty$, $\mathbf{h} \to 0$ or $\mathbf{h} \to 0$, $L \to \infty$ as required on general grounds[8] for $O(n)$ invariant quantities.

3. Critical Behavior

So far we have not yet dealt with the critical ($r_0 \to r_{0c}$, $\mathbf{h} \to 0$) behavior of $P(\mathbf{\Phi})$. For this purpose we turn to renormalized field theory (by performing the limit $\Lambda \to \infty$ at fixed renormalized parameters) employing dimensional regularization and minimal subtraction at fixed $d < 4$.[9] The renormalized quantities are as usual $\varphi_R = Z_\varphi^{-1/2}\varphi$, $u = \mu^{-\varepsilon} A_d Z_u^{-1} Z_\varphi^2 u_0$, and $r = Z_r^{-1}(r_0 - r_{0c}) = at$ where r_{0c} is the (bulk) critical value of r_0 and A_d is a convenient geometrical factor with $A_3 = (4\pi)^{-1}$. In general it is also necessary to renormalize the external field according to $\mathbf{h}_R = Z_\varphi^{1/2}\mathbf{h}$. Using the notation $P(\mathbf{\Phi}) \equiv P(r_0 - r_{0c}, \mathbf{h}, u_0, L, \mathbf{\Phi})$ for the bare distribution function Eq. (5) we introduce the renormalized distribution function

$$P_R(r, \mathbf{h}_R, u, \mu, L, \mathbf{\Phi}_R) = Z_\varphi^{n/2} P(Z_r r, Z_\varphi^{-1/2}\mathbf{h}_R, \mu^\varepsilon Z_u Z_\varphi^{-2} A_d^{-1} u, L, Z_\varphi^{1/2}\mathbf{\Phi}_R) . \tag{24}$$

Most important is the fact that *the new fourth-order terms $H_k^{(4)}$ in H_1 do not cause new ultraviolet ($\Lambda \to \infty$) divergencies beyond one-loop order* as can be shown by studying the large-$\mathbf{k}$, i.e. large-$\mathbf{m}$ contributions to Eq. (21). Thus it suffices to renormalize H^{eff} by the standard Z factors in one-loop order although H^{eff} contains arbitrary large powers of Φ^2 and u_0/L^{d-4}. The details of the (multiplicative) renormalization of H^{eff} will be given elsewhere.[10] The distribution function Eq. (24) satisfies the renormalization-group equation

$$\left[\mu\frac{\partial}{\partial\mu}+\beta_u\frac{\partial}{\partial u}+\zeta_r r\frac{\partial}{\partial r}+\frac{1}{2}\zeta_\varphi\left(n+\mathbf{\Phi}_{\mathrm{R}}\frac{\partial}{\partial\mathbf{\Phi}_{\mathrm{R}}}-\mathbf{h}_{\mathrm{R}}\frac{\partial}{\partial\mathbf{h}_{\mathrm{R}}}\right)\right]P_{\mathrm{R}}=0 \qquad (25)$$

where β_u, ζ_r and ζ_φ are the usual field-theoretic functions.[9] Integration of this equation yields

$$P_{\mathrm{R}}(r,\mathbf{h},u,L,\mu,\mathbf{\Phi}_{\mathrm{R}})=P_{\mathrm{R}}(r(\ell),\mathbf{h}_{\mathrm{R}}(\ell),u(\ell),L,\mu\ell,\mathbf{\Phi}_{\mathrm{R}}(\ell))\times\exp\left[-\frac{n}{2}\int_\ell^1\zeta_\varphi(u(\ell'))\frac{d\ell'}{\ell'}\right], \qquad (26)$$

where ℓ is the flow parameter and

$$\mathbf{\Phi}_{\mathrm{R}}(\ell)=\mathbf{\Phi}_{\mathrm{R}}\exp\left[-\frac{1}{2}\int_\ell^1\zeta_\varphi(u(\ell'))\frac{d\ell'}{\ell'}\right], \qquad (27)$$

$$\mathbf{h}_{\mathrm{R}}(\ell)=\mathbf{h}_{\mathrm{R}}\exp\left[\frac{1}{2}\int_\ell^1\zeta_\varphi(u(\ell'))\frac{d\ell'}{\ell'}\right]. \qquad (28)$$

At this point the question arises of how to choose ℓ. For a detailed discussion of this question see Ref. 3. Here we only recall that for $\mathbf{h}=0$ an appropriate choice of ℓ is made[6] by requiring $\mu^2\ell^2$ to be equal to the effective renormalized counterpart of $r_0+12u_0M_0^2$. A simple and appropriate way of taking the critical $\mathbf{h}$ dependence into account[3] is to choose $\ell(t,L,h)$ by requiring $\mu^2\ell^2$ to be equal to the effective renormalized counterpart of $r_0+12u_0M_0^2(h)$ where

$$M_0^2(h)=Z_0(\mathbf{h})^{-1}\int d^n\mathbf{\Phi}\Phi^2e^{-H_0(\mathbf{\Phi},\mathbf{h})}, \qquad (29)$$

$$Z_0(\mathbf{h})=\int d^n\mathbf{\Phi}e^{-H_0(\mathbf{\Phi},\mathbf{h})} \qquad (30)$$

with $H_0(\mathbf{\Phi},\mathbf{h})$ given by Eq. (8). Following Ref. 11 we perform the integration over the angular coordinates of $\mathbf{\Phi}$ to obtain

$$M_0^2(h)=(L^du_0)^{-1/2}\,\vartheta_2(y_0,q_0) \qquad (31)$$

where

$$\vartheta_2(y_0,q_0)=\frac{\int_0^\infty ds s^{n+1}\zeta_n(q_0s)\exp(-(1/2y_0)s^2-s^4)}{\int_0^\infty ds s^{n-1}\zeta_n(q_0s)\exp(-(1/2y_0)s^2-s^4)} \qquad (32)$$

with the dimensionless parameters

$$y_0 = r_0 L^{d/2} u_0^{-1/2}, \tag{33}$$

$$\mathbf{q}_0 = \mathbf{h} L^{3d/4} u_0^{-1/4}. \tag{34}$$

The n-dependent function $\zeta_n(q_0 s)$ arising from the angular integration is given by[11]

$$\zeta_n(q_0 s) = \Gamma\left(\frac{n}{2}\right)\left(\frac{2}{q_0 s}\right)^{(n-2)/2} I_{(n/2)-1}(q_0 s) \tag{35}$$

where $\Gamma(z)$ and $I_\nu(y)$ denote the standard gamma function and Bessel function of the imaginary argument, respectively.[12,13] (For $q_0 = 0$ we have $\zeta_n(0) = 1$ and $\vartheta_2(y_0, 0) = \vartheta_2(y_0)$ as in Ref. 6.) The requirement mentioned above leads to the following implicit equation determining $\ell(t, L, h)$,

$$r(\ell) + 12(\mu\ell)^{\varepsilon/2} A_d^{-1/2} u(\ell)^{1/2} L^{-d/2} \vartheta_2(y(\ell), \hat{q}(\ell)) = \mu^2 \ell^2 \tag{36}$$

with the dimensionless effective parameters

$$y(\ell) = r(\ell)(\mu\ell)^{-2}(\mu\ell L)^{d/2} A_d^{1/2} u(\ell)^{-1/2}, \tag{37}$$

$$\hat{\mathbf{q}}(\ell) = \mathbf{h}_R(\ell)(\mu\ell)^{-(d/2)-1}(\mu\ell L)^{3d/4} A_d^{1/4} u(\ell)^{-1/4}, \tag{38}$$

which is the h dependent generalization of Eqs. (5.15)–(5.17) of Ref. 6. Asymptotically (small ℓ, i.e., large L, small $|t|$, small $|\mathbf{h}|$), we obtain from Eqs. (21)–(24), (26), (36)–(38) the finite-size scaling form

$$P(\mathbf{\Phi}, t, \mathbf{h}, L) = L^{n\beta/\nu} f(\mathbf{\Phi} L^{\beta/\nu}, t L^{1/\nu}, \mathbf{h} L^{\beta\delta/\nu}). \tag{39}$$

The resulting scaling function has the structure

$$f(\mathbf{z}, x, \mathbf{q}) = \frac{\exp[-F(\mathbf{z}, x, \mathbf{q})]}{\int d^n\mathbf{z} \exp[-F(\mathbf{z}, x, \mathbf{q})]}, \tag{40}$$

with $\mathbf{z} = \mathbf{\Phi} L^{\beta/\nu}$, $x = t L^{1/\nu}$, $\mathbf{q} = \mathbf{h} L^{\beta\delta/\nu}$ and

$$\begin{aligned} F(\mathbf{z}, x, \mathbf{q}) = {} & c_2(\hat{x}, q)\hat{z}^2 + c_4(\hat{x}, q)\hat{z}^4 - \mathbf{q}\cdot\mathbf{z} \\ & - \frac{1}{2}\sum_{\mathbf{m}\neq 0} \ln\left\{\frac{Z_1[y_{\mathbf{m}}(\tilde{r}_L(\hat{z}, \hat{x}, q))]}{Z_1[y_{\mathbf{m}}(\tilde{r}_L(0, \hat{x}, q))]}\right\} \\ & - \frac{1}{2}(n-1)\sum_{\mathbf{m}\neq 0} \ln\left\{\frac{Z_1[y_{\mathbf{m}}(\tilde{r}_T(\hat{z}, \hat{x}, q))]}{Z_1[y_{\mathbf{m}}(\tilde{r}_T(0, \hat{x}, q))]}\right\}. \end{aligned} \tag{41}$$

Here $\hat{x} = Q^* t(L/\xi_0)^{1/\nu}$ and $\hat{z} = (2Q^*)^\beta (\Phi/A_M)(L/\xi_0)^{\beta/\nu}$ are convenient dimensionless scaling variables normalized to the asymptotic amplitudes A_M and ξ_0 of the bulk order-parameter $M_{\text{bulk}} = A_M|t|^\beta$ at $h = 0$ below T_c and of the bulk correlation length $\xi = \xi_0 t^{-\nu}$ at $h = 0$ above T_c. The well-known bulk parameter $Q^*(n)$[9] will be given below. In three dimensions we obtain

$$y_{\mathbf{m}}(\tilde{r}(\hat{z}, \hat{x}, q)) = [6\pi u^* \tilde{\ell}(\hat{x}, q)]^{-1/2} [\tilde{r}(\hat{z}, \hat{x}, q)\tilde{\ell}(\hat{x}, q)^2 + 4\pi^2 \mathbf{m}^2] , \tag{42}$$

$$\tilde{r}_L(\hat{z}, \hat{x}, q) = \hat{x}\tilde{\ell}(\hat{x}, q)^{-1/\nu} + (3/2)\tilde{\ell}(\hat{x}, q)^{-2\beta\nu}\hat{z}^2 , \tag{43}$$

$$\tilde{r}_T(\hat{z}, \hat{x}, q) = \hat{x}\tilde{\ell}(\hat{x}, q)^{-1/\nu} + (1/2)\tilde{\ell}(\hat{x}, q)^{-2\beta\nu}\hat{z}^2 , \tag{44}$$

which are the dimensionless renormalized counterparts of $y_{0\mathbf{m}}$, $r_{0L} - r_{0c}$, and $r_{0T} - r_{0c}$, respectively. The coefficients $c_2(\hat{x}, q)$ and $c_4(\hat{x}, q)$ read for $d = 3$

$$c_2(\hat{x}, q) = (64\pi u^*)^{-1} \hat{x}\tilde{\ell}(\hat{x}, q)^{3-(2\beta+1)/\nu} [1 + 4(n+2)u^*] , \tag{45}$$

$$c_4(\hat{x}, q) = (256\pi u^*)^{-1} \tilde{\ell}(\hat{x}, q)^{3-4\beta/\nu} [1 + 4(n+8)u^*] , \tag{46}$$

where $u^*(n)$ is the known[9] fixed point value of the renormalized coupling u. The auxiliary scaling function $\tilde{\ell}(\hat{x}, q) = \mu L \ell(t, L, h)$ of the flow parameter is determined by Eqs. (36)–(38) which yield asymptotically, in 3 dimensions,

$$\tilde{\ell}(\hat{x}, q)^{3/2} = (4\pi u^*)^{1/2} [\tilde{y}(\hat{x}, q) + 12\vartheta_2(\tilde{y}(\hat{x}, q), \tilde{q})] , \tag{47}$$

$$\tilde{y}(\hat{x}, q) = (4\pi u^*)^{-1/2} \tilde{\ell}(\hat{x}, q)^{3/2-1/\nu} \hat{x} , \tag{48}$$

$$\tilde{q} = A_M (2Q^*)^{-\beta} \xi_0^{\beta/\nu} (4\pi u^*)^{1/4} \sqrt{8}\tilde{\ell}(\hat{x}, q)^{\beta/\nu - 3/4} q . \tag{49}$$

Note that, apart from the linear term $-\mathbf{q}\cdot\mathbf{z}$ in Eq. (41), the additional q dependence in all other terms originates from the h dependent choice of the flow parameter according to Eqs. (36) and (47) through the function $\vartheta_2(\tilde{y}, \tilde{q})$. In particular, at $T = T_c$ and $L = \infty$ we obtain from (47)–(49), $\ell \sim h^{\nu/\beta\delta}$ as expected on the basis of scaling. The sums $\sum_{\mathbf{m}\neq 0}$ in Eq. (41) can be evaluated by using the prescriptions of dimensional regularization[14] and by computing their finite contributions in three dimensions numerically.[10]

In a comparison with MC data of spin models our result for the universal function $f(\mathbf{z}, x, \mathbf{q})$ requires no additional adjustment of nonuniversal parameters, i.e. we need to adjust only the *bulk* amplitudes A_M and ξ_0 at $h = 0$.

4. Quantitative Predictions and Comparison with MC Data

In this section we present quantitative predictions of our theory and compare them with MC data of O(n) symmetric 3D spin models for $n = 1, 2, 3$.

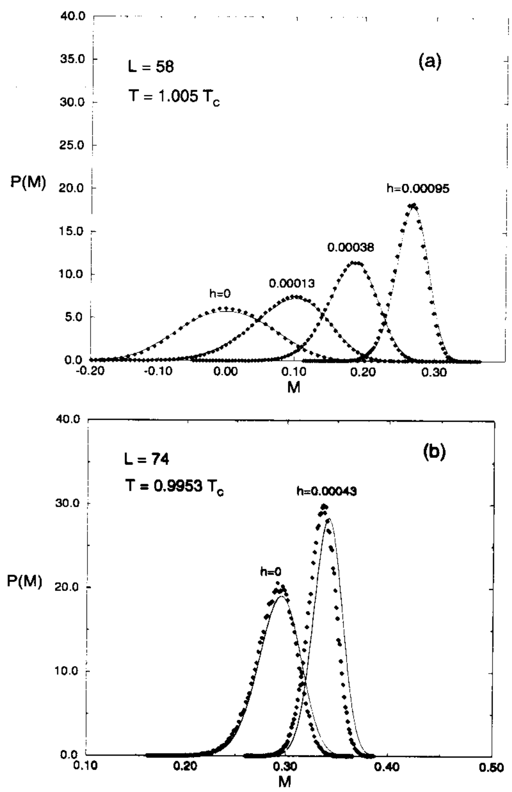

Fig. 1. Distribution function $P(M)$ for the (dimensionless) magnetization $M = \Phi\tilde{a}^{1/2}$ (with $\tilde{a}$ being the lattice constant) of the $L \times L \times L$ Ising model for several values of the (dimensionless) magnetic field $\tilde{h} = h\tilde{a}^{5/2}$: (a) above T_c at $t = T/T_c - 1 = 0.005$ and $\tilde{h} = 0$, $\tilde{h} = 0.00013$, 0.00038, 0.00095 for $L = 58\tilde{a}$ and (b) below T_c at $t = -0.0047$ and $\tilde{h} = 0$, $\tilde{h} = 0.00043$ for $L = 74\tilde{a}$. MC data are from Ref. 15. Solid lines are the theoretical result obtained from (38)–(49). The normalization is $\int_{-\infty}^{\infty} dM\, P(M) = 1$.

In Figs. 1(a) and (b) we compare our result (39)–(49), in units of the lattice constant $\tilde{a}$, with the MC data of the 3D Ising model by Tsypin[15] for several values of the dimensionless external field $\tilde{h} = h\tilde{a}^{5/2}$ above and below T_c. From Ref. 6, we have taken $u^*(1) = 0.0412$, $Q^*(1) = 0.945$, and from Ref. 16, $\xi_0/\tilde{a} = 0.495$, $A_M\tilde{a}^{1/2} = 1.71$, $\beta = 0.3305$, $\nu = 0.6335$. We see that there is excellent agreement between our theory and the MC data.

In Figs. 2(a)–(c) we illustrate the predictions of our theory for the finite-size scaling function (40)–(49) near the (rounded) first-order transition of the finite 3D Ising model below T_c. At $h = 0$ (Fig. 2(a)), the scaling function has two symmetric peaks. For small $hL^{\beta\delta/\nu}$ (Fig. 2(b)), the system starts to develop an asymmetric distribution function whose asymmetry becomes more pronounced as $hL^{\beta\delta/\nu}$ increases.[3] The peak for the magnetization along the direction of **h** increases while that for the magnetization opposite to **h** decreases. Finally the latter peak essentially disappears for $\tilde{h}(L/\tilde{a})^{\beta\delta/\nu} \gtrsim 2$ (Fig. 2(c)). This explains why in the case

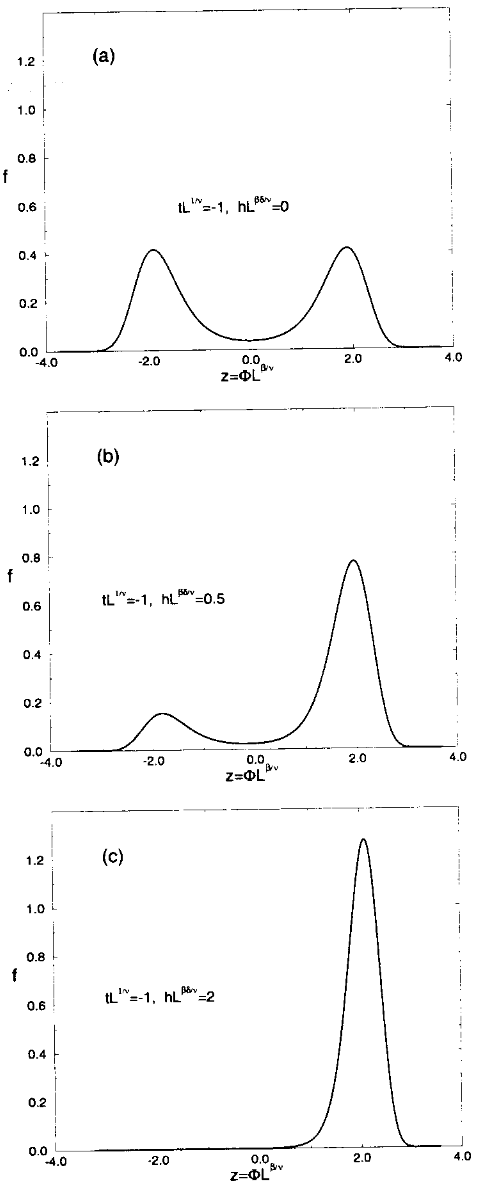

Fig. 2. Theoretical prediction for the finite-size scaling function of the 3D Ising model according to (40)–(49) versus the scaled dimensionless magnetization $z = \Phi\tilde{a}^{1/2}(L/\tilde{a})^{\beta/\nu}$ for three values of the scaled dimensionless magnetic field in the range $0 \leq h\tilde{a}^{5/2}(L/\tilde{a})^{\beta\delta/\nu} \leq 2.0$ below T_c at $x = t(L/\tilde{a})^{1/\nu} = -1$. The normalization is $\int_{-\infty}^{\infty} dz f(z,x,q) = 1$.

of $\tilde{h} = 0.00043$, $L/\tilde{a} = 74$ shown in Fig. 1(b) (corresponding to the large value $\tilde{h}(L/\tilde{a})^{\beta\delta/\nu} = 18.45$) there is only one peak left. In the bulk limit, the distribution functions at fixed $\mathbf{h} \neq \mathbf{0}$ become single-peaked δ-functions which then imply a sharp first-order transition as $\mathbf{h}$ changes sign.

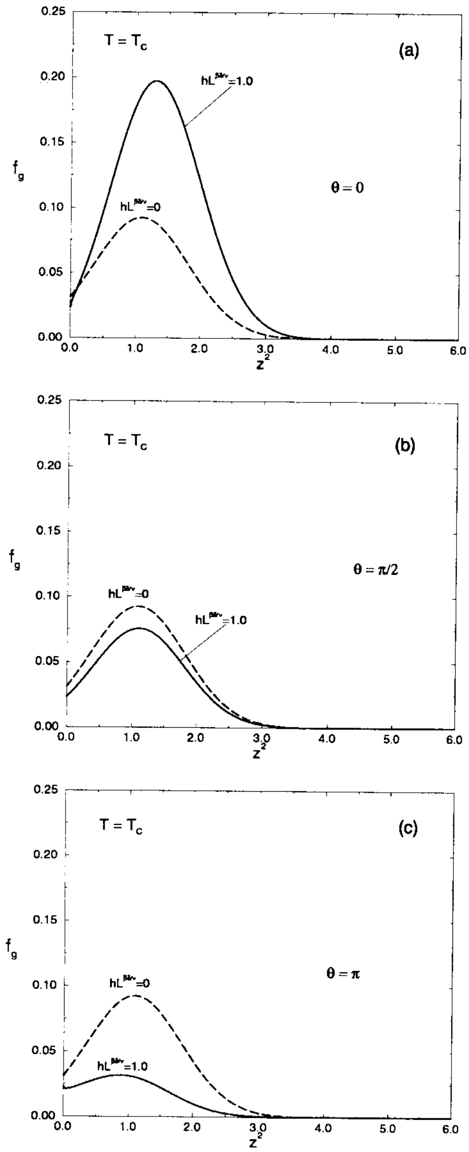

Fig. 3. Theoretical prediction for the finite-size scaling function $f_g(\mathbf{z}, 0, \mathbf{q})$ (solid lines) of the 3D XY model at $T = T_c$ according to (40)–(49) and (51) versus the square z^2 of the dimensionless scaled magnetization $\mathbf{z} = \mathbf{\Phi}\tilde{a}^{1/2}(L/\tilde{a})^{\beta/\nu}$ at fixed scaled magnetic field $h\tilde{a}^{5/2}(L/\tilde{a})^{\beta\delta/\nu} = 1$ for three angles θ between the direction of $\mathbf{h}$ and of $\mathbf{\Phi}$: (a) $\theta = 0$ ($\mathbf{\Phi}$ parallel to $\mathbf{h}$), (b) $\theta = \pi/2$ ($\mathbf{\Phi}$ perpendicular to $\mathbf{h}$), (c) $\theta = \pi$ ($\mathbf{\Phi}$ antiparallel to $\mathbf{h}$). The dashed lines represent f_g at $h = 0$. The normalization is $\int_0^{2\pi} d\theta \int_0^{\infty} d(z^2) f_g(\mathbf{z}, 0, \mathbf{q}) = 1$.

In Figs. 3(a)–(c) we show the results of our theory for the case $n = 2$ at $T = T_c$ at finite $\mathbf{h}$. For future tests by means of MC simulations for the 3D XY-model we have chosen the bulk parameters as $\beta = 0.344$,[17] $\nu = 0.671$,[18] $u^*(2) = 0.0362$,

$Q^*(2) = 0.939$,[9] $\xi_0/\tilde{a} = 0.498$,[19] $A_M \tilde{a}^{1/2} = 1.217$.[2] In the presence of the external field $\mathbf{h}$ the scaling function $f(\mathbf{z}, x, \mathbf{q})$ now depends on the angle θ between the magnetization $\mathbf{\Phi}$ and $\mathbf{h}$. Because of the normalization condition

$$\int d^2\mathbf{z} f(\mathbf{z}, x, \mathbf{q}) = \int_0^{2\pi} d\theta \int_0^{\infty} d(z^2) \frac{1}{2} f(\mathbf{z}, x, \mathbf{q}) = 1 \tag{50}$$

we have plotted in Figs. 3(a)–(c) the scaling function

$$f_g(\mathbf{z}, 0, \mathbf{q}) = \frac{1}{2} f(\mathbf{z}, 0, \mathbf{q}) \tag{51}$$

at fixed value of the scaled magnetic field $|\mathbf{h}|\tilde{a}^{5/2}(L/\tilde{a})^{\beta\delta/\nu} = 1.0$ (i.e. at fixed $\mathbf{q}$) as a function of the dimensionless scaling variable $z^2 = \Phi^2 \tilde{a}(L/\tilde{a})^{2\beta/\nu}$ for three angles θ from $\theta = 0$ ($\mathbf{\Phi}$ being parallel to $\mathbf{h}$) to $\theta = \pi$ ($\mathbf{\Phi}$ being antiparallel to $\mathbf{h}$). (For $\theta = \pi/3$ and $2\pi/3$ see Ref. 3.) The dashed line represents the case $h = 0$ which is independent of θ. We see that, at finite $\mathbf{h}$, the scaling function exhibits an interesting dependence on the magnitude and direction of the magnetization relative to $\mathbf{h}$ which can be tested by MC simulations.

Finally we compare in Fig. 4 our results for $h = 0$ with MC data for the 3D XY and 3D Heisenberg models.[2] Since, at $h = 0$, $f(z, x, 0)$ depends only on $|z|$ (rather than on the vector $\mathbf{z}$) and because of $d^n z = g(n) d(|z|^n)$ with $g(n) = 2\pi^{n/2}[n\Gamma(n/2)]^{-1}$ we have plotted $f_g(z, x, 0) = g(n) f(z, x, 0)$ versus $|z|^n$ in Fig. 4 for $n = 2$ and 3. The corresponding values of the bulk parameters for $n = 3$ are $Q^* = 0.937$, $u^* = 0.0328$[9]; for the bulk critical exponents we take $\beta = 0.365$, $\nu = 0.705$.[17,20] (For the bulk parameters for $n = 2$ see above.)

Figure 4 shows that the MC data for various lattice sizes are in good agreement with the theoretical predictions both at T_c and below T_c. (Similar agreement is found above T_c.) The different steepness of f at T_c near $z = 0$ for $n = 2$ and $n = 3$ is well described by the theory. The qualitative difference between the increasing ($n = 2$) and decreasing ($n = 3$) maximum below T_c is an unexpected n-dependence of the order-parameter distribution function.

Having established the shape of $f(\mathbf{z}, x, \mathbf{q})$ we are in the position to determine the finite-size effects on various important thermodynamic quantities such as susceptibility, specific heat, and magnetization (equation of state). A generalization to different geometries and boundary conditions can also be studied. Our idea of a non-perturbative treatment of the $\mathbf{k} \neq 0$ modes may also open up the possibility of entering the unexplored area of finite-size *dynamics* of $O(n)$ symmetric systems below T_c.[22] Finally we note that this idea also constitutes a new approach to bulk perturbation theory for the long-distance properties of $O(n)$ symmetric systems below T_c. Work in this direction is in progress.

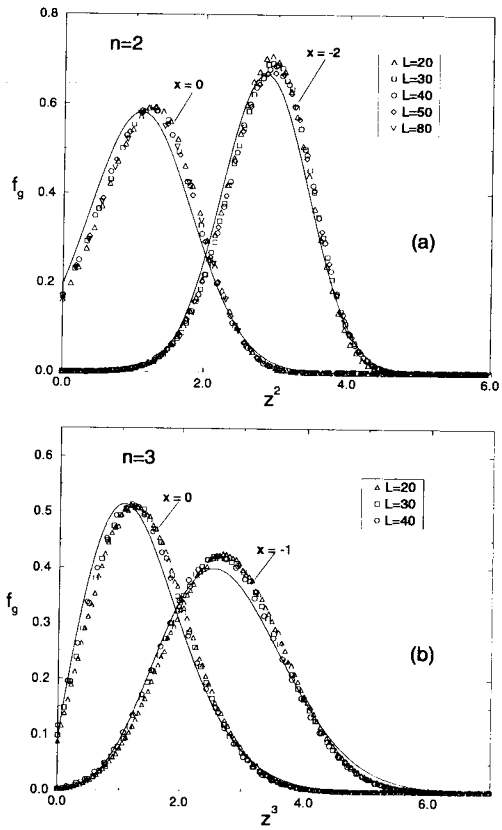

Fig. 4. Theoretical predictions (solid lines) and MC data for the scaling function $f_g(z, x, 0) = g(n)f(z, x, 0)$ at T_c ($x = 0$) and below T_c ($x < 0$): (a) for the XY model ($\xi_0 = 0.498$, $A_M = 1.217, g(2) = \pi$) and (b) for the Heisenberg model ($\xi_0 = 0.484$,[21] $A_M = 1.118$, $g(3) = 4\pi/3$), with $z = \Phi L^{\beta/\nu}$ and $x = tL^{1/\nu}$, in units of the lattice constant. MC data are from Ref. 2. The normalization is $\int_0^\infty f_g(z, x, 0) d(|z|^n) = 1$.

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