Calculation of subcritical exponents for corrections to scaling

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The "subcritical" exponent Δ_{2s} for corrections to asymptotic scaling in the renormalization-group theory of critical phenomena, has been calculated for the continuous-spin versions of the classical, $d=3$ Ising, X-Y, and Heisenberg models by numerical integrations of Wilson's approximate recursion formula. The results are $\Delta_{2s}(\text{Ising}) = -0.640$, $\Delta_{2s}(X\text{-}Y) = -0.644$, and $\Delta_{2s}(\text{Heisenberg}) = -0.647$. Comparison is made with results from perturbation expansions in $\epsilon = 4 - d$ (d being the dimensionality), high-temperature series expansions, and experimental measurements.

Wegner has shown[1] that the presence of irrelevant operators, and their conjugate fields, in the renormalization-group theory of critical phenomena implies that near criticality the singular part of the free-energy density will be a generalized homogeneous function of an infinite set of scaling fields $(\mu_1, \mu_2, \mu_3, \ldots)$:

$$F_s(\mu_1, \mu_2, \mu_3, \ldots) = l^{-d} F_s(l^{y_1}\mu_1, l^{y_2}\mu_2, l^{y_3}\mu_3, \ldots) . \tag{1}$$

The scaling fields are all expected to be analytic functions of the thermodynamic fields. For ordinary critical points only two of the fields, μ_1 and μ_2, are relevant ($y_1 > y_2 > 0 > y_3 > y_4 \cdots$) and must vanish at criticality. Thus, Widom's well-known scaling hypothesis is regained as $l \to \infty$, μ_1 and $\mu_2 \to 0$.

The irrelevant fields are manifested in terms of a nonanalytic background for the leading critical-point anomalies. For the isotropic spin models[2] which are often used to describe the critical phenomena in many real systems, including fluids, superfluid ^{4}He and isotropic ferro- and antiferromagnets, the dominant contribution to this nonanalytic background comes from the "2s" operator, the first irrelevant operator with full spin rotational symmetry. Thus, for example, one expects the isothermal susceptibility of a ferromagnet at $H=0$ to display a critical anomaly of the form[1]

$$\chi_T \simeq \mathcal{T}^{-\gamma}(A + B\mathcal{T}^{-\Delta_{2s}} + \cdots) \tag{2}$$

while the density difference of the liquid-gas coexistence curve is expected to vanish near criticality as[3]

$$\rho_L - \rho_G \simeq \mathcal{T}^{\beta}(a + b\mathcal{T}^{-\Delta_{2s}} + \cdots) , \tag{3}$$

where $\mathcal{T} = (T - T_c)/T_c$, the coefficients A, a, B, and b are analytic functions of $\mathcal{T}$, the Δ_{2s} is equal to $y_{2s}\nu$, and the $\cdots$ represent less pronounced background anomalies from the other irrelevant fields with $y_i < y_{2s}$.

Under favorable circumstances it may be possible to obtain quantitative information about the nonanalytic background terms, either experimentally[4] or from the analysis of series-expansion data.[5] Such information would offer a useful test of the renormalization-group theory for corrections to scaling. It is also possible that the background terms may be significant in the analysis of experimental data for the accurate determination of the form of the leading critical-point singularity. Therefore it seems important to attempt to calculate the exponent Δ_{2s} directly from the renormalization-group theory.

Thus far, the only systematic investigations of this problem have been based on the very elegant method of perturbation expansions in $\epsilon = 4 - d$, where d is the dimensionality.[6] This scheme has been carried out to third order[7,8] in ϵ for n-dimensional spins in $d = 4 - \epsilon$ space dimensions. The numerical results for $d = 3$ ($\epsilon = 1$) are given at orders ϵ, ϵ^2, and ϵ^3 in the first three data columns of Table I. It can be seen that the presently available ϵ expansion for Δ_{2s} is very erratic. This type of behavior, although especially pronounced in the present case, is a commonly observed feature of the ϵ-expansion approach.[9]

An alternative general method for calculating critical and subcritical exponents in the renormalization group theory may be based upon numerical investigations of Wilson's $\eta = 0$ recursion relation.[10] This approach offers, in effect, an approximate resummation of the ϵ expansion, which includes contributions from all orders in ϵ by introducing simplifying assumptions in the evalua-

tion of terms of order ϵ^2 and higher.[6] A major defect of the approximate recursion relation is apparently the constraint that the critical exponent η must vanish, whereas one typically finds $\eta \leq 0.05$ for $d=3$. The $\eta=0$ recursion formula has been used in the past to calculate critical exponents and other critical parameters for the classical $d=3$ Ising,[10] X-Y,[11] and Heisenberg models.[12] We report here on the calculation of the subcritical exponent Δ_{2s} for these models.

Wilson's formulation in the $\eta=0$ approximation leads to an effective Hamiltonian for spin fluctuations of wave vector $|\vec{k}|<2^{-p}$, p an integer, of the form

$$H_p[\vec{s}(\vec{x})] = -\int [|\vec{\nabla}\vec{s}(\vec{x})|^2 + Q_p(\vec{s}(\vec{x}))]d\vec{x}. \tag{4}$$

Hamiltonians for different wave-vector, or wavelength, cutoffs are related by a nonlinear integral recursion operator $Q_{p+1}(\vec{z}) = R[Q_p(\vec{z})]$ where

$$R[Q(\vec{z})] = -2^d \ln\left(\int_{-\infty}^{\infty} d\vec{y}\exp[-\vec{y}\cdot\vec{y} - \tfrac{1}{2}Q(2^{1-d/2}\vec{z}+\vec{y}) - \tfrac{1}{2}Q(2^{1-d/2}\vec{z}-\vec{y})] \Big/ \int_{-\infty}^{\infty} d\vec{y}\exp[-\vec{y}\cdot\vec{y} - Q(y)]\right). \tag{5}$$

At the critical point the correlation length for spin fluctuations becomes infinite and the sequence $\{Q_p(\vec{z})\}$ of effective Hamiltonians of longer and longer minimum wavelength, generated by iteration of R, is found to go to a limit, or fixed point, $Q^*(\vec{z})$.

The scaling exponents $\{y_i\}$ are determined by the stability properties of $Q^*(\vec{z})$. Linearization of R about $Q^*(\vec{z})$ defines a spectrum of eigenfunctions $\{\psi_i(\vec{z})\}$ and eigenvalues $\{\lambda_i = 2^{y_i}\}$. The scaling fields $\{\mu_i\}$ of (1) are defined by the decomposition

$$Q_0(\vec{z}) = Q^*(\vec{z}) + \sum_i \mu_i \psi_i(\vec{z}) \tag{6}$$

with some normalization for the $\{\psi_i(\vec{z})\}$. For isotropic $Q^*(\vec{z})$ the eigenfunctions may be classified,[7] like hydrogenic orbitals, according to the irreducible representations of the spin rotation group. This leads to the notation $y_i = y_{n,l}$ with $n = 0, 1, 2, \ldots$ and $l = s, p, d, \ldots$.

In performing the calculations with (5), one represents the recursion operator by an approximate numerical algorithm, and the fixed point and stability properties of this algorithm are then determined by iteration on a computer. The functions $Q(|\vec{z}|)$ are specified for $0 \leq |\vec{z}| \leq 4.0$ on a 41-point mesh. Lagrange interpolation is used between the mesh points and a $|\vec{z}|^6$ extrapolation is assumed for $|\vec{z}| > 4.0$. The Ising and X-Y model integrals are performed by Simpson's rule and the Heisenberg model by trapezoidal rule. For the Ising model the integration variable y is varied from 0.0 to 4.0 with a 41-point mesh. For the X-Y model the variable $|\vec{y}|$ is varied in the same manner and $\theta = \arccos(\vec{z}\cdot\vec{y})/|\vec{z}|\cdot|\vec{y}|$ is varied from 0.0 to $\frac{1}{2}\pi$ on a 32-point mesh. For the Heisenberg model the integration variables are essentially $|\vec{z}/\sqrt{2} + \vec{y}|$ and $|\vec{z}/\sqrt{2} - \vec{y}|$ on a mesh of spacing $\Delta = 0.1$ and going out to $|\vec{z}|, |\vec{y}| = 4.0$. This choice of variables reduces the three-dimensional integration to a pair of one-dimensional integrals.

TABLE I. Predictions for Δ_{2s}.

Model	$O(\epsilon)$	$O(\epsilon^2)$	$O(\epsilon^3)$	This work
Ising	−0.5	−0.269	−1.068	−0.640
X-Y	−0.5	−0.300	−1.014	−0.644
Heisenberg	−0.5	−0.329	−0.969	−0.647

Starting with a function $Q_0(r, \vec{z}) = r|\vec{z}|^2 + 0.5|\vec{z}|^4$, one obtains an estimate, λ_{1s}^e, of the relevant s-type eigenvalue and, $Q_e^*(\vec{z})$, of the fixed point by constructing a series $\{r_p\}$ such that $Q_p(r_p, \vec{z}) = R^p[Q_0(r_p, \vec{z})]$ has a specified value, zero, at some value of $\vec{z}$, $|\vec{z}| = 1.5$. Then $\{r_p\}$ tends to a limit as $r_p \simeq r_c + a\lambda_{1s}^{-p}$ and $Q_p(r_c, \vec{z})$ tends to $Q^*(\vec{z})$ for large p. This procedure does not converge rapidly in practice and an improved estimate of $Q^*(\vec{z})$ is obtained from the elimination, for $l \sim 5, 6$

$$Q_e^*(\vec{z}) \leftarrow R^l[Q_e^*(\vec{z})] + \frac{1}{1-\lambda_{1s}^e}\{R^{l+1}[Q_e^*(\vec{z})] - R^l[Q_e^*(\vec{z})]\}. \tag{7}$$

The effects of small errors in the estimate of $Q^*(\vec{z})$ is further reduced in practice by numerically constructing the linearization of (5) for small perturbations, $\psi(\vec{z})$, about $Q^*(\vec{z})$ in the form $\psi_{p+1}(\vec{z}) = \mathcal{L}\psi_p(\vec{z})$ with

$$\mathcal{L}\psi(\vec{z}) = R[Q_e^*(\vec{z}) + \psi(\vec{z})] - R[Q_e^*(\vec{z})]. \tag{8}$$

Given an s-type starting function $[\psi(\vec{z}) = \psi(|\vec{z}|) \sim 10^{-3}]$, repeated operation of $\mathcal{L}$ and division by λ_{1s}^e eventually yields an estimate, $\psi_{1s}^e(\vec{z})$, of the $1s$ eigenfunction. With each further iteration of $\mathcal{L}$ this function becomes multiplied by a factor of λ_{1s}, thus allowing a more accurate determination of the eigenvalue. This improved estimate of λ_{1s} may then be used to further improve the estimate $Q_e^*(\vec{z})$ through the elimination procedure (7). The process is iterated until an estimate of $Q^*(\vec{z})$ is obtained which changes by less than one part in 10^6 (in the worst case, X-Y model) with each

iteration. It should be emphasized that this type of accuracy in the determination of $Q^*(\vec{z})$, and elsewhere, is necessary in order to be able to study the $2s$ eigenfunction, which would otherwise be obscured by rapidly growing $1s$-type errors. The estimates of λ_{1s} obtained are $\lambda_{1s}(\text{Ising}) \simeq 3.1203$, $\lambda_{1s}(X\text{-}Y) \simeq 2.9321$, and $\lambda_{1s}(\text{Heisenberg}) \simeq 2.7796$, implying $y_{1s}(\text{Ising}) \simeq 1.642$, $y_{1s}(X\text{-}Y) \simeq 1.552$, and $y_{1s}(\text{Heisenberg}) \simeq 1.475$.

Using the best estimates for $Q^*(\vec{z})$ and λ_{1s}, repeatedly operating by $\mathfrak{L}$, and dividing the result by λ_{1s} yields an estimate of the $1s$ contribution to any starting s-type function $\psi(|\vec{z}|) \sim 10^{-3}$. This estimate is subtracted from $\psi(|\vec{z}|)$ to obtain a new starting function $\bar{\psi}(|\vec{z}|)$, and the entire process is repeated as many times as necessary to yield a result which is, for all practical purposes, orthogonal to $\psi_{1s}(|\vec{z}|)$. The value of λ_{2s} is then determined by repeatedly operating on this new function with the linearized recursion $\mathfrak{L}$. One observes, with the first few iterations, an erratic behavior due to the other more rapidly decaying irrelevant perturbations. This is followed by a period of regular behavior during which the iterated function is simply scaled by a factor of λ_{2s} from each iteration of $\mathfrak{L}$. This behavior then breaks down due to the rapidly growing, small $1s$-type errors present.

The values of λ_{2s} obtained in this manner are $\lambda_{2s}(\text{Ising}) \simeq 0.483$, $\lambda_{2s}(X\text{-}Y) \simeq 0.499$, and $\lambda_{2s}(\text{Heisenberg}) \simeq 0.516$. This yields $y_{2s}(\text{Ising}) \simeq -1.05$, $y_{2s}(X\text{-}Y) \simeq -1.00$, and $y_{2s}(\text{Heisenberg}) \simeq -0.955$. Finally for $\Delta_{2s} = y_{2s}/y_{1s} = y_{2s}\nu$ one obtains $\Delta_{2s}(\text{Ising}) \simeq -0.640$, $\Delta_{2s}(X\text{-}Y) \simeq -0.644$ and $\Delta_{2s}(\text{Heisenberg}) \simeq -0.647$. These values are listed in the fourth data column of Table I.

It is interesting to note that both y_{2s} and Δ_{2s} are found to depend only weakly upon the dimensionality of the spin vector. This is also a prediction of the first-order ϵ expansion which always gives $\Delta_{2s} = -0.5$. The calculated values for y_{2s} are also quite close to the universal value, $y_{2s} = -1.0$, obtained at $O(\epsilon)$; however, the predictions for Δ_{2s} are substantially different, as the relation $\Delta_{2s} = y_{2s}\nu$ involves, at $O(\epsilon)$, the mean field value $\nu = \frac{1}{2}$. There is no obvious relation between our numerical results and the higher-order ϵ expansions. We finally mention that by the same techniques we have also been able to obtain an estimate of the eigenvalue $\lambda_{2p}(\text{Ising})$, corresponding to the first irrelevant operator with p-type symmetry. Our result is $\lambda_{2p}(\text{Ising}) \simeq 0.1$ to 0.2. This is in qualitative agreement with Wegner's calculation to first order in ϵ which gives $\lambda_{2p}(\text{Ising}) = \frac{1}{8}$ for $d = 3$.

There is presently very little known from other sources concerning the value of Δ_{2s}. From the analysis of Ising-model series data,[5] Wortis has predicted $\Delta_{2s} \sim -0.5$. From experimental data on the superfluid transition in ^{4}He, Ahlers has estimated[4] $-0.5 \geq \Delta_{2s} \geq -0.9$. It is our hope that the results of the calculations described here will offer more reliable estimates of the quantity Δ_{2s} which will be of value in the future in connection with the detailed analysis of experimental and series-expansion data for critical-point anomalies.

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