The Scaling Functions of the Free Energy Density and its Derivatives for the $3d\ O(4)$ Model

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Preprint BI-TP 2011/06, arXiv: 1105.0584[hep-lat]

Overview:

- Introduction and Motivation
- Model and Observable Definition
- Critical Behaviour and Scaling Functions
- Determination of Parameters from Data
- Scaling Tests for ϵ and C, the Non-singular Part of ϵ
- Summary

Introduction and Motivation

- A scaling function of an observable describes the general critical behaviour near a continuous phase transition. It is a universal function for all members of a universality class, just like the critical exponents.

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- If the scaling function of the free energy density is known, the scaling functions of all its derivatives (for the observables $M, \chi_L, \epsilon, C, \ldots$) can be calculated. In principle, only one of these scaling functions and the critical exponents are needed to perform a (nearly) complete test on the universality class.

  The most used and discussed scaling function is that of the magnetization M. It is part of the magnetic equation of state (EOS).

  $\Longrightarrow$ This scaling function is known for the $3d\ O(4)$ model!

Examples:

D. Toussaint, Phys. Rev. D55 (1997) 362
F. P. Toldin, A. Pelissetto and E. Vicari, JHEP 07 (2003) 289
A. Cucchieri and T. Mendes, J. Phys. A38 (2005) 4561
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However:

All existing parametrizations of this function are not well suited for a comparison to data. Instead they are used to calculate another form of scaling function. Taking derivatives of this second form with the then indirect parametrization is cumbersome. This is also true for our own (old) parametrization, for example for the comparison to susceptibility data.

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Therefore: Parametrize directly the second form, then it is easy to

- Perform scaling tests for ϵ and C, which involve such derivatives. Only problem: the non-singular contributions.
- Calculate pseudocritical lines from extrema of scaling functions of the second kind (important for QCD).

In addition: The QCD community is interested in even higher T-derivatives to estimate cumulants of baryon number fluctuations near T_c

The $3d$ $O(4)$ Model and the Observables

We use the standard $O(4)$-invariant non-linear σ model

$$\beta\mathcal{H} \;=\; -J \sum_{<\vec{x},\vec{y}>} \vec{\phi}_{\vec{x}} \cdot \vec{\phi}_{\vec{y}} \;-\; \vec{H} \cdot \sum_{\vec{x}} \vec{\phi}_{\vec{x}}$$

$\vec{\phi}_{\vec{x}}$ is a 4-component unit vector at site $\vec{x}$ on a $3d$ cubic lattice, $\vec{\phi}_{\vec{x}}^{\,2} = 1$.

J and the external field $\vec{H}$ are reduced quantities: they contain each a factor $\beta = 1/T$.

Indentify directly: $J \equiv 1/T$

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Decompose $\vec{\phi}_{\vec{x}}$ in longitudinal, $\parallel$ to $\vec{H}$, and transverse, $\perp$ to $\vec{H}$, components

$$\vec{\phi}_{\vec{x}} = \phi^{\parallel}_{\vec{x}} \vec{e}_H + \vec{\phi}^{\perp}_{\vec{x}} \;, \quad \vec{e}_H = \vec{H}/H$$

Lattice average of longitudinal spin components, $L =$ No. of lattice points per direction

$$\varphi^{\parallel} = \frac{1}{V} \sum_{\vec{x}} \phi^{\parallel}_{\vec{x}} \;, \quad V = L^3$$

The $3d\ O(4)$ Model and the Observables

Energy of a spin configuration

$$E = -\sum_{<\vec{x},\vec{y}>} \vec{\phi}_{\vec{x}} \cdot \vec{\phi}_{\vec{y}}$$

Partition function

$$Z(T,H) = \int \prod_{\vec{x}} d^4\phi_{\vec{x}}\,\delta(\vec{\phi}^{\,2}_{\vec{x}} - 1)\ \exp(-\beta E + HV\varphi^{\|}) = \exp(-\beta F)$$

$F =$ free energy and (reduced) free energy density

$$f(T,H) = \frac{\beta F}{V} = -\frac{1}{V}\ln Z$$

The Observables measured on the Lattice

First and second partial derivatives of $f(T,H)$:

Magnetization	$M = -\frac{\partial f}{\partial H} = \langle \varphi^{\parallel} \rangle$
Longitudinal susceptibility	$\chi_L = \frac{\partial M}{\partial H} = V(\langle \varphi^{\parallel 2} \rangle - M^2)$
Energy density	$\epsilon = \frac{\partial f}{\partial \beta} = \frac{\langle E \rangle}{V}$
Specific heat	$C = \frac{\partial \epsilon}{\partial T} = \frac{\beta^2}{V}(\langle E^2 \rangle - \langle E \rangle^2)$
Thermal susceptibility	$\chi_t = \frac{\partial M}{\partial \beta} = \langle E \rangle \langle \varphi^{\parallel} \rangle - \langle E \varphi^{\parallel} \rangle$

Critical Behaviour and Scaling Functions

Leading terms of the scaling laws, thermodynamic limit

$t = (T - T_c)/T_c$, critical point: $t = 0, H = 0$

$t < 0, H = 0,$ low T phase

$$\begin{aligned} M &= B(-t)^{\beta} \\ \chi_L &\to \infty \quad \text{Goldstone effect} \\ \chi_t &= \beta B T_c (-t)^{\beta - 1} \end{aligned}$$

$t > 0, H = 0,$ high T phase

$$\begin{aligned} M &= 0 \\ \chi_L &= C^{+} t^{-\gamma} \\ \chi_t &= 0 \end{aligned}$$

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$$M = 0$$
$$\chi_L = C^{+} t^{-\gamma}$$
$$\chi_t = 0$$

Energy density and specific heat

$$\epsilon = \epsilon_{ns} + \frac{A^{\pm}}{\alpha(1-\alpha)} T_c t |t|^{-\alpha}$$
$$C = C_{ns} + \frac{A^{\pm}}{\alpha} |t|^{-\alpha}$$

Critical Behaviour and Scaling Functions

$t = 0, H > 0,$ critical isotherm

$$M = B^c H^{1/\delta} \Leftrightarrow H = D_c M^\delta$$

Historical relation, reason for δ

$$\chi_L = C^c H^{1/\delta - 1}\,, \quad C^c = \frac{B^c}{\delta}$$

$$\chi_t = X_c H^{(\beta-1)/\Delta}\,, \quad \Delta = \beta\delta = \beta + \gamma$$

"gap exponent" $2 - \alpha - \Delta = \beta$

$\beta - \Delta = -\gamma$

$$\epsilon = \epsilon_{ns} + E_c H^{(1-\alpha)/\Delta}$$

$$C = C_{ns} + \frac{A_c}{\alpha_c} H^{-\alpha_c}\,, \quad \alpha_c = \frac{\alpha}{\Delta}\,,$$

$$\frac{1}{\delta} = \beta_c\,, \quad \frac{1}{\delta} - 1 = -\gamma_c$$

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$$\epsilon = \epsilon_{ns} + E_c H^{(1-\alpha)/\Delta}$$

$$C = C_{ns} + \frac{A_c}{\alpha_c} H^{-\alpha_c}, \quad \alpha_c = \frac{\alpha}{\Delta},$$

$$\frac{1}{\delta} = \beta_c, \quad \frac{1}{\delta} - 1 = -\gamma_c$$

Free energy density f consists of two parts:

f_s = singular part, responsible for critical behaviour

f_{ns} = non-singular (regular) part, background

Assumption: $f(T, H) = f_s(T, H) + f_{ns}(T)$

The Free Energy Density

Other opinions:

V. Privman et al. , Domb and Lebowitz, Eds. , Vol.14 (1991):

f_{ns} can be chosen to be H-independent.

A. Pelissetto and E. Vicari, Phys. Rep. 368 (2002) 549:

$$f_{ns} = f_{ns}(T, H)$$

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$$f_{ns} = c_{H2}H^2 + c_{J1}t + c_{J2}t^2 + c_{J3}t^3$$

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The scaling laws for M and χ_L:

$$\frac{\partial f_{ns}}{\partial H}(T, H = 0) = \frac{\partial^2 f_{ns}}{\partial H^2}(T, H = 0) = 0 \,, \quad \frac{\partial f_{ns}}{\partial H}(T_c, H) = \frac{\partial^2 f_{ns}}{\partial H^2}(T_c, H) = 0 \,.$$

$$\hookrightarrow \qquad \epsilon = \epsilon_{ns}(T) + \epsilon_s(T, H) \,, \quad C = C_{ns}(T) + C_s(T, H)$$

Expansion of $\epsilon_{ns}(T)$ at $T = T_c$, though T_c is not a distinguished point of it:

$$\epsilon_{ns}(T) = \epsilon_{ns}(T_c) + (T - T_c) \cdot C_{ns}(T_c) + \frac{1}{2}(T - T_c)^2 \cdot C'_{ns}(T_c) + \ldots$$

The Scaling Functions

Generalization of scaling laws to non-zeo t and H

Historically, before RG theory (1965/67):

$$H(T,M) = M|M|^{\delta-1}\Phi_H(t|M|^{-1/\beta})$$

Widom-Griffiths (WG) form of the equation of state,
Φ_H is universal, if 2 normalization conditions are imposed.

The thermodynamic variables T, H are here replaced by the set of variables T, M, by starting from the Gibbs free energy G instead of the free energy F. In terms of the reduced free energy densities

$$g = f + MH$$

However, we want to compare with MC-data for M at fixed T, H.

Unfortunately: all field theory calculations use the WG-form, and also usually the normalized function Φ_H is parametrized!

RG Theory: the Scaling Equation for f_s

$$f_s(u_1, u_2, u_3, \dots) = b^{-d} f_s(b^{y_1} u_1, b^{y_2} u_2, b^{y_3} u_3, \dots)$$

$u_j =$ scaling fields, $b =$ positive scale factor, $y_j =$ RG eigenvalues

$3d\ O(4)$ class: 2 relevant scaling fields $y_1 = y_t, y_2 = y_h > 0$

$j > 2$: irrelevant scaling fields with $y_j < 0$

$y_t = 1/\nu\ ,\ y_h = 1/\nu_c = \Delta/\nu\ ,\ \Delta = y_h/y_t$

Close to the critical point: $u_t = c_t t\ ,\ u_h = c_h H$

$c_t, c_h =$ model-dependent (positive) metric scale factors

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Different forms of scaling functions:

They are obtained by different choices for b

1. form: $b^{y_t}|u_t| = 1$

$$f_s(u_t, u_h, u_{j>2}) \ = \ |u_t|^{d/y_t} f_s(\pm 1, u_h |u_t|^{-y_h/y_t}, u_j |u_t|^{-y_j/y_t})$$

$$f_s(u_t, u_h) \ = \ (c_t |t|)^{d/y_t} \Psi_{1\pm}(c_h c_t^{-\Delta} H |t|^{-\Delta})$$

The last equation is valid close to the critical point. By solving the corresponding M-equation for H one obtains the WG-form.

Forms of Scaling Functions

2. form: $b^{y_h}|u_h| = 1$

$$f_s(u_t, u_h) = (c_h|H|)^{d/y_h}\Psi_{2\pm}(c_t c_h^{-1/\Delta}\, t|H|^{-1/\Delta})$$

$\Psi_{2\pm} = \Psi_2$, independent of sgn$H$

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$\Psi_{2\pm} = \Psi_2$, independent of sgn$H$

3. form: $(b^{y_t}t)^2 + (b^{y_h}H)^2 = 1$

The equation can be solved numerically for $b = b(t, H) > 0$,

and with $\theta(t, H) = \arctan\ (b^{y_h}H/b^{y_t}t)$ one finds

$$f_s = -b(t, H)^{-d} g_T(\theta(t, H))$$

Toussaint parametrized the function $g_T(\theta)$.

All forms are of course equivalent!

The Magnetic Equation of State

Instead of working with c_t, c_h one imposes two constraints on the scaling function for M by introducing new variables ($H > 0$ in the following)

$$\bar{t} = (T - T_c)/T_0 = tT_c/T_0 \; , \quad h = H/H_0$$

such that

$$M(T = T_c) = h^{1/\delta} \implies H_0 = D_c = (B^c)^{-\delta}$$
$$M(H = 0) = (-\bar{t}\,)^{\beta} \implies T_0 = B^{-1/\beta} T_c$$

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WG-form:

$$y = f(x) \ , \quad x = \bar{t} M^{-1/\beta} \ , \quad y = h/M^{\delta}$$
$$f(0) = 1 \ , \quad f(-1) = 0$$

2. form:

$$M = h^{1/\delta} f_G(z) \ , \quad z = \bar{t} h^{-1/\Delta}$$
$$f_G(0) = 1 \ , \quad f_G(z) \underset{z \to -\infty}{\longrightarrow} (-z)^{\beta}$$

Connection:

$$f_G = y^{-1/\delta} \ , \quad z = x y^{-1/\Delta}$$

In the following we use the second form for all observables!

The 2. Form Scaling Equations

We start from the scaling equation for f_s with the corresponding scaling function $f_f(z)$

$$f_s = H_0 h^{1+1/\delta} f_f(z)$$

Since $M = -\partial f_s / \partial H = h^{1/\delta} f_G(z)$ we have the differential equation

$$f_G(z) = -(1 + \frac{1}{\delta}) f_f(z) + \frac{z}{\Delta} f_f'(z)$$

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The scaling equations for the other observables:

$$\chi_L = \frac{h^{\frac{1}{\delta}-1}}{H_0} f_\chi(z) \quad \text{with} \quad f_\chi(z) = \frac{1}{\delta} f_G(z) - \frac{z}{\Delta} f_G'(z)$$

$$\epsilon_s = -T^2 \frac{H_0}{T_0} h^{(1-\alpha)/\Delta} f_f'(z)\,, \qquad C_s - \frac{2\epsilon_s}{T} = -\left(\frac{T}{T_0}\right)^2 H_0 h^{-\alpha/\Delta} f_f''(z)$$

$$\chi_t = -\frac{T^2}{T_0} h^{(\beta-1)/\Delta} f_G'(z)$$

Representation of the Scaling Functions

f_s is not a direct observable. However, we can use the magnetization data to find $f_G(z)$. Once we have parametrized $f_G(z)$ we can solve the differential equation for $f_f(z)$ (DE).

Representation of $f_G(z)$ and $f_f(z)$ in terms of 3 expansions:

a power series for small z , and 2 asymptotic expansions for $z \to \pm\infty$

1. small z

$$f_f(z) = \sum_{n=0}^{\infty} a_n z^n \; , \quad f_G(z) = \sum_{n=0}^{\infty} b_n z^n$$

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$$\mathrm{DE}: \qquad b_n = \left[-(1 + \frac{1}{\delta}) + \frac{n}{\Delta} \right] a_n \quad \Longrightarrow \quad a_n = \frac{\Delta b_n}{\alpha + n - 2} \ ,$$

Here, $1 + 1/\delta = (2 - \alpha)/\Delta$ and because of the normalization

$$f_G(0) = 1 = b_0 \ , \quad \Longrightarrow \quad f_f(0) = \frac{\Delta}{\alpha - 2} = a_0$$

Representation of the Scaling Functions

2. $z \to +\infty$ corresponds to $t > 0$ and $H \to 0$, high temperature region
Leading term of $f_G(z)$ is $\sim z^{-\gamma}$, the same as that of $f_\chi(z)$

$$\chi_L = \frac{h^{-\gamma/\Delta}}{H_0} f_\chi(z) \underset{z\to+\infty}{=} C^+ t^{-\gamma} \, , \quad \Longrightarrow \quad f_\chi(z) \underset{z\to+\infty}{\longrightarrow} z^{-\gamma} C^+ D_c B^{\delta-1} = R_\chi z^{-\gamma}$$

For $t > 0$, M is an odd function of H, $M \sim H$ – Griffiths's condition

Therefore:

$$f_G(z) = z^{-\gamma} \sum_{n=0}^{\infty} d_n^+ z^{-2n\Delta} \, , \qquad d_0^+ = R_\chi$$

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Ansatz for $f_f(z)$:

$$f_f(z) = z^{2-\alpha} \sum_{n=0}^{\infty} c_n^+ z^{-2n\Delta}$$

$$\mathrm{DE}: \qquad c_{n+1}^+ = \frac{-d_n^+}{2(n+1)} \,, \qquad c_1^+ = -\frac{R_\chi}{2} \,,$$

however, c_0^+ is not specified!

Representation of the Scaling Functions

3. $z \to -\infty$ corresponds to $t < 0$ and $H \to 0$, low temperature region
Leading term of $f_G(z)$ is $= (-z)^\beta$, normalization!

For $t < 0$ we have massless Goldstone modes and

$$\chi_L(T < T_c, H) \sim H^{-1/2} \text{ for small H} \implies M(T < T_c, H) = (-\bar{t}\,)^\beta + m_1 H^{1/2} + \ldots$$

Therefore:

$$f_G(z) = (-z)^\beta \sum_{n=0}^{\infty} d_n^- (-z)^{-n\Delta/2}\,, \qquad d_0^- = 1$$

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$$\text{DE}: \qquad c_{n+2}^- = \frac{-2d_n^-}{n+2} \,, \qquad c_1^- \equiv 0 \,, \; c_2^- = -1 \,,$$

however, c_0^- is not specified!

Final Solution of the Differential Equation

How to find $c_0^{\pm}$? $\alpha < 0$ for the $3d\ O(4)$ class:

a) $z > 0$, small z expansion

$$\sum_{n=3}^{\infty} a_n z^n = \Delta \sum_{n=3}^{\infty} \frac{b_n z^n}{\alpha + n - 2} = \Delta z^{2-\alpha} \int_0^z dy y^{\alpha-3} \sum_{n=3}^{\infty} b_n y^n$$

$$= \Delta z^{2-\alpha} \int_0^z dy y^{\alpha-3} \left[f_G(y) - 1 - b_1 y - b_2 y^2 \right]$$

$$= f_f(z) - a_0 - a_1 z - a_2 z^2$$

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$$= f_f(z) - a_0 - a_1 z - a_2 z^2$$

$$c_0^+ = \lim_{z\to\infty} f_f(z) z^{\alpha-2} = \Delta \int_0^{\infty} dy y^{\alpha-3} \left[f_G(y) - 1 - b_1 y - b_2 y^2 \right]$$

Partial integration:

$$c_0^+ = \frac{\Delta}{2-\alpha} \int_0^{\infty} dy y^{\alpha-2} \left[f_G'(y) - f_G'(0) - y f_G''(0) \right]$$

Final Solution of the Differential Equation

b) $z < 0$, same procedure

$$f_f(z) = a_0 + a_1 z + a_2 z^2 + \Delta(-z)^{2-\alpha} \int_z^0 dy(-y)^{\alpha-3} \left[f_G(y) - 1 - b_1 y - b_2 y^2 \right]$$

$$c_0^- = \frac{-\Delta}{2-\alpha} \int_{-\infty}^0 dy(-y)^{\alpha-2} \left[f'_G(y) - f'_G(0) - y f''_G(0) \right]$$

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$$c_0^- = \frac{-\Delta}{2-\alpha} \int_{-\infty}^0 dy(-y)^{\alpha-2} \left[f_G'(y) - f_G'(0) - y f_G''(0)\right]$$

$f_f(z)$ is universal as a whole, and also the $c_0^\pm$. They are universal products of critical amplitudes

$$c_0^\pm = f_s^\pm (B^c)^\delta B^{-(1+\delta)}$$

Here, the $f_s^\pm$ are the critical amplitudes of the free energy density for $H = 0,\ t \neq 0$

$$f = f_{ns}(T) + f_s^\pm |t|^{2-\alpha} \text{ , and } f_s^\pm = \frac{A^\pm}{-\alpha(1-\alpha)(2-\alpha)} \text{ , } \Longrightarrow \quad \frac{A^+}{A^-} = \frac{c_0^+}{c_0^-}$$

Determination of Parameters from Data

Data from: J. E. and O. Vogt, Nucl. Phys. B832 (2010) 538
Simulation on $L = 120$ lattice with cluster algorithm of
U. Wolff, Phys. Rev. Lett. 62 (1989) 361

$0.90 \le J = 1/T \le 1.2 \; ; \quad 0.0001 \le H \le 0.007$

$J_c = 0.93590 \; , \quad 10^5$ measurements at fixed J, H

Finite size effects: none for ϵ, for M only at $H = 0.0001$,
more for χ_L, χ_t and C

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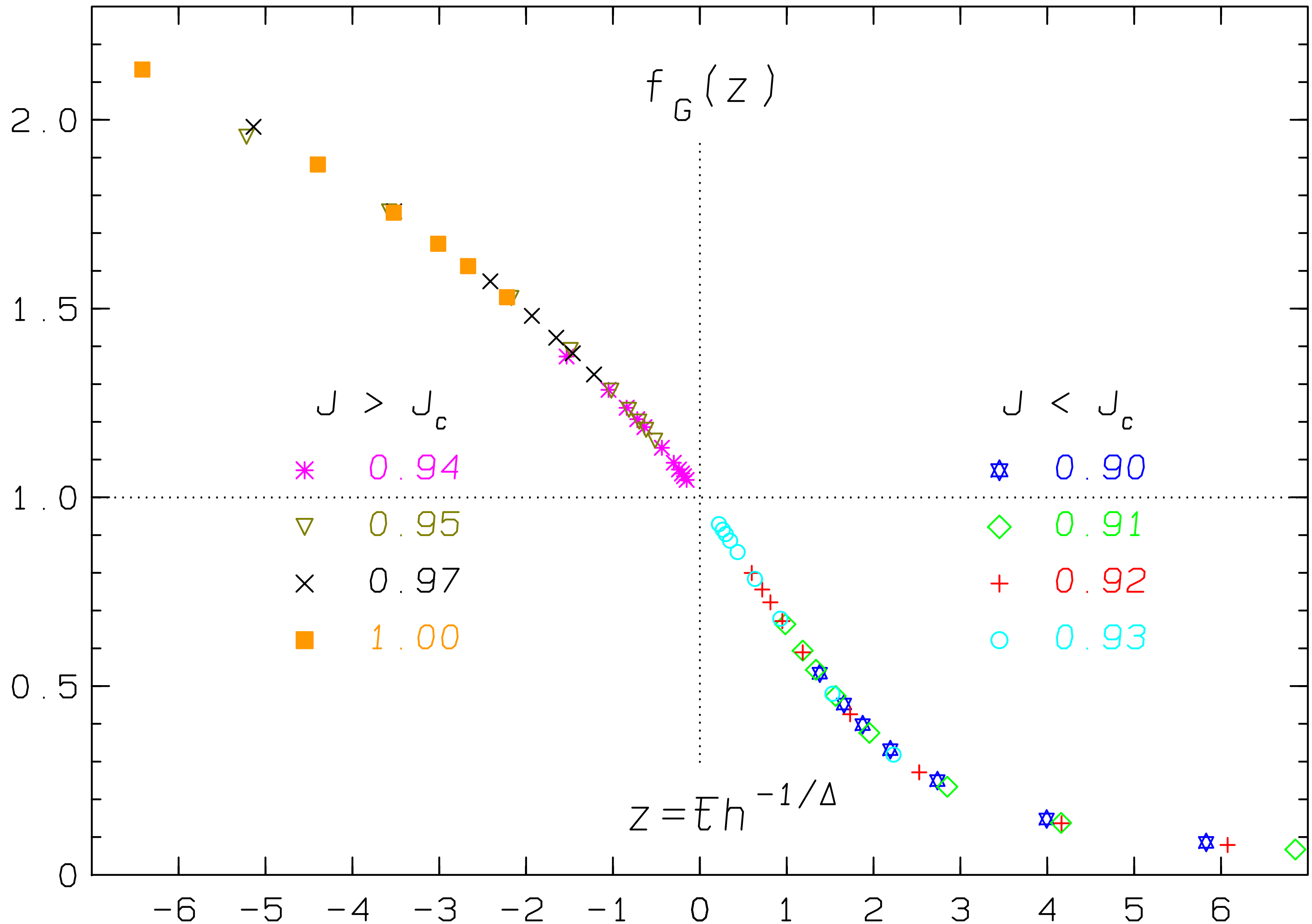
Possible problem in calculating $f_G(z)$: corrections-to-scaling .
They appear at larger $|t|$ and H-values, depending on the special model

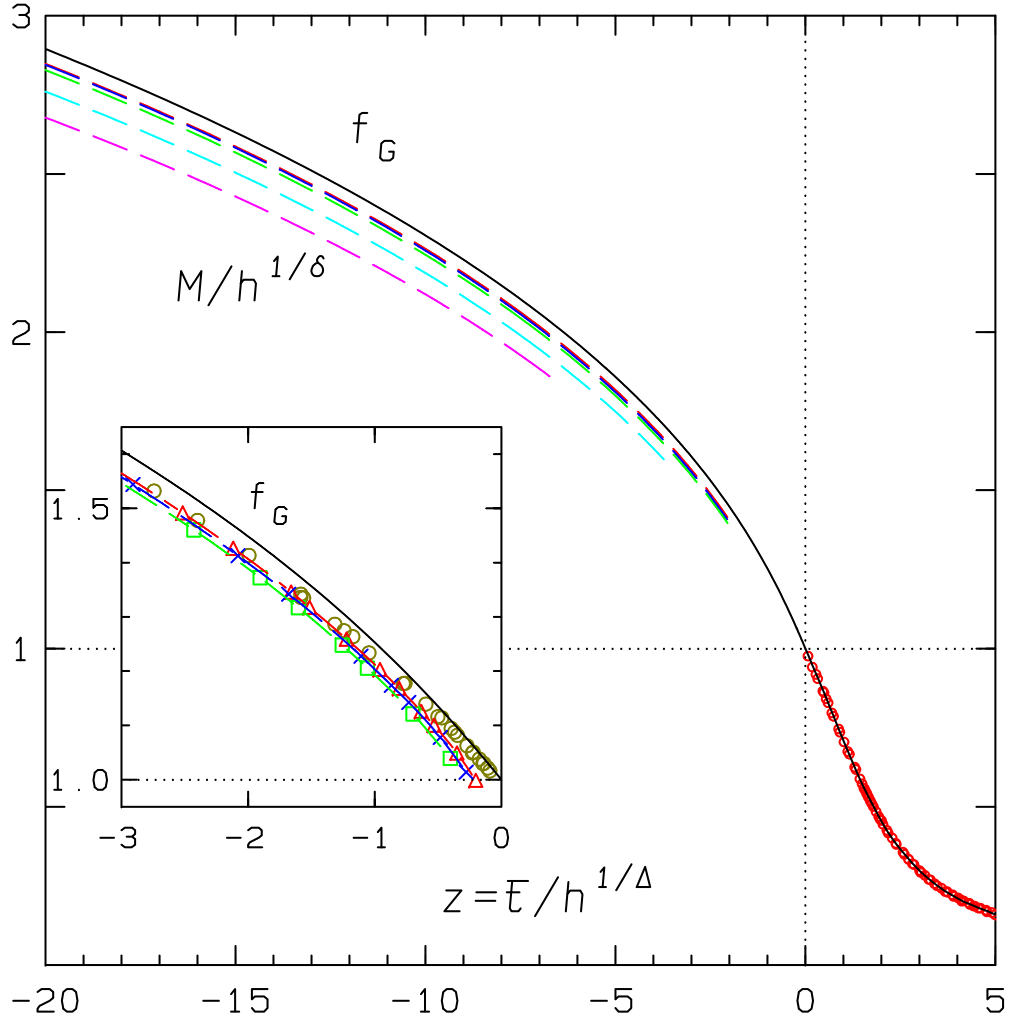
Fortunately: we find perfect scaling properties for $Mh^{-1/\delta} = f_G(z)$ in our model and for our values of $|t|$ and H ,

Counterexample: the $O(2)$-symmetric non-linear σ-model shows strong scaling violations for $z < 0$ $(t < 0)$

Data for the scaling function $f_G(z)$ from M



Data for $f_G(z)$ in the $O(2)$-symmetric non-linear σ-model



J. E. , S. Holtmann, T. Mendes, T. Schulze, Phys. Lett. B492 (2000) 219

Corrections-to-scaling

Explanation for the difference between $O(2)$ and $O(4)$ by

M. Hasenbusch and T. Török, J. Phys. A32 (1999) 6361 ($N = 2$)
M. Hasenbusch, J. Phys. A34 (2001) 8221 ($N = 4$)

$\Longrightarrow$ Leading corrections to scaling can be eliminated by using instead of the $O(N)$-invariant non-linear model the respective $O(N)$-invariant ϕ^4 model, where $\beta\mathcal{H}$ contains in addition the term $\sum_x [\lambda(\vec{\phi}_x^2 - 1)^2 + \vec{\phi}_x^2]$, and tuning the new parameter λ. Optimal values:

$\lambda = 2.1$ for $N = 2$, $\lambda = 12.5(4.0)$ for $N = 4$, our case: $\lambda = \infty$

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In order to plot $f_G(z)$ and to define $t,\bar{t},h$ and z one needs T_c,T_0,H_0 and the critical exponents. We use the values of

J. E. , L. Fromme, M. Seniuch, Nucl. Phys. B675 (2003) 533

The corresponding exponent values are close to the field theory results of

R. Guida and J. Zinn-Justin, J. Phys. A31 (1998) 8103

see also M. Hasenbusch $(N=4)$ above

Parametrization in 3 Steps

1. Fit of f_G-data ($f_G = Mh^{-1/\delta}$) in the asymptotic regimes with the first 3 terms each. We discard the $H = 0.0001$-data for $z < 0$. Fit ranges: $z < 0 : \; [-10, -1]$ and $z > 0 : \; [1.5, 15]$

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2. Fit of $-f'_G(z)$ in the small z-region, instead of f_G, because there is a peak , which one can hardly see in f_G. The $-f'_G(z)$-data are obtained from two sources:

$$-f'_G = \frac{T_0}{T^2} h^{-(\beta-1)/\Delta} \cdot \chi_t$$

$$-f'_G = \frac{\Delta}{z}(\delta f_\chi - f_G) = \frac{\Delta}{z} h^{-1/\delta} [\delta H \chi_L - M]$$

$\Longrightarrow$ $f_G(z)$ is parametrized.

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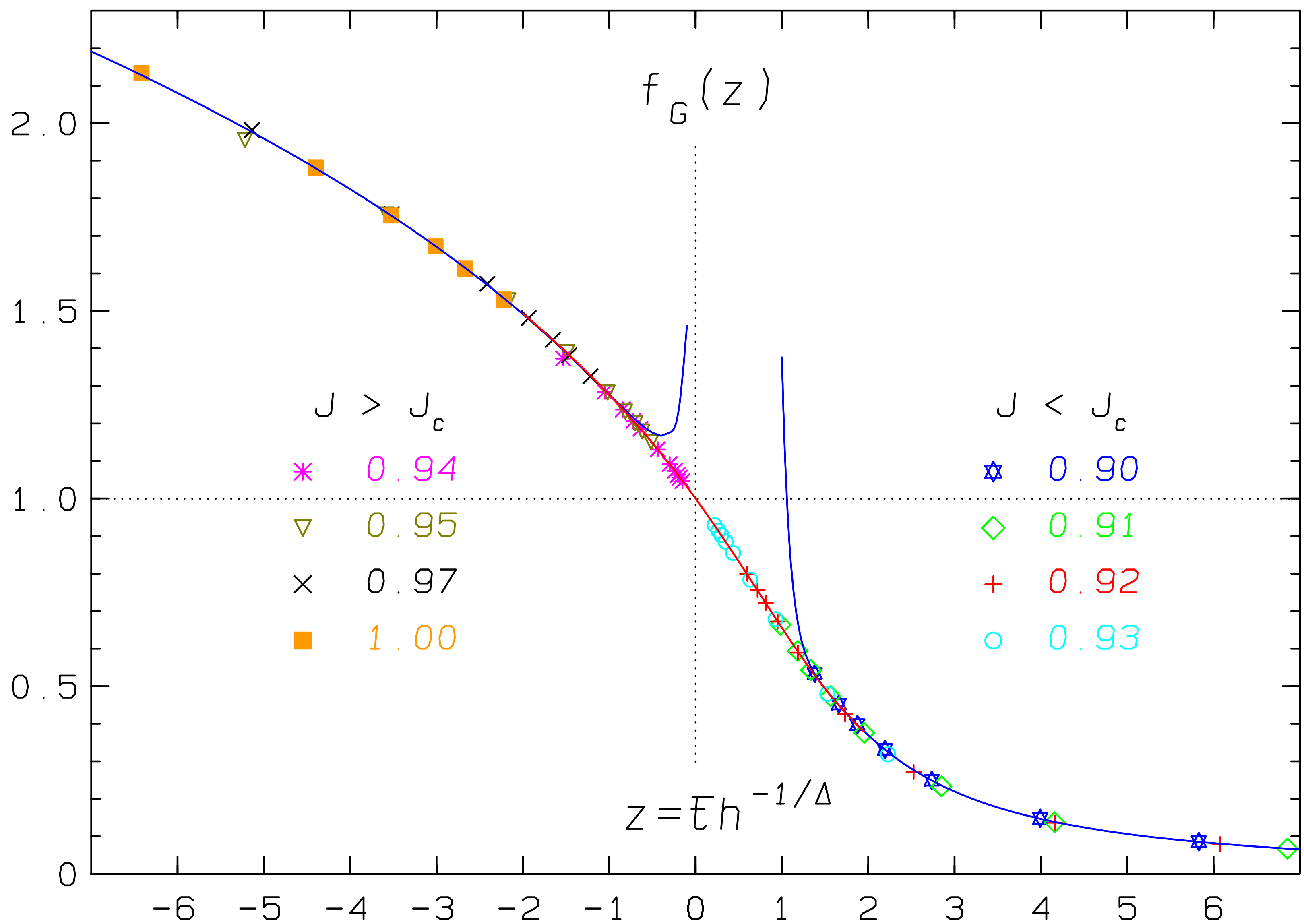
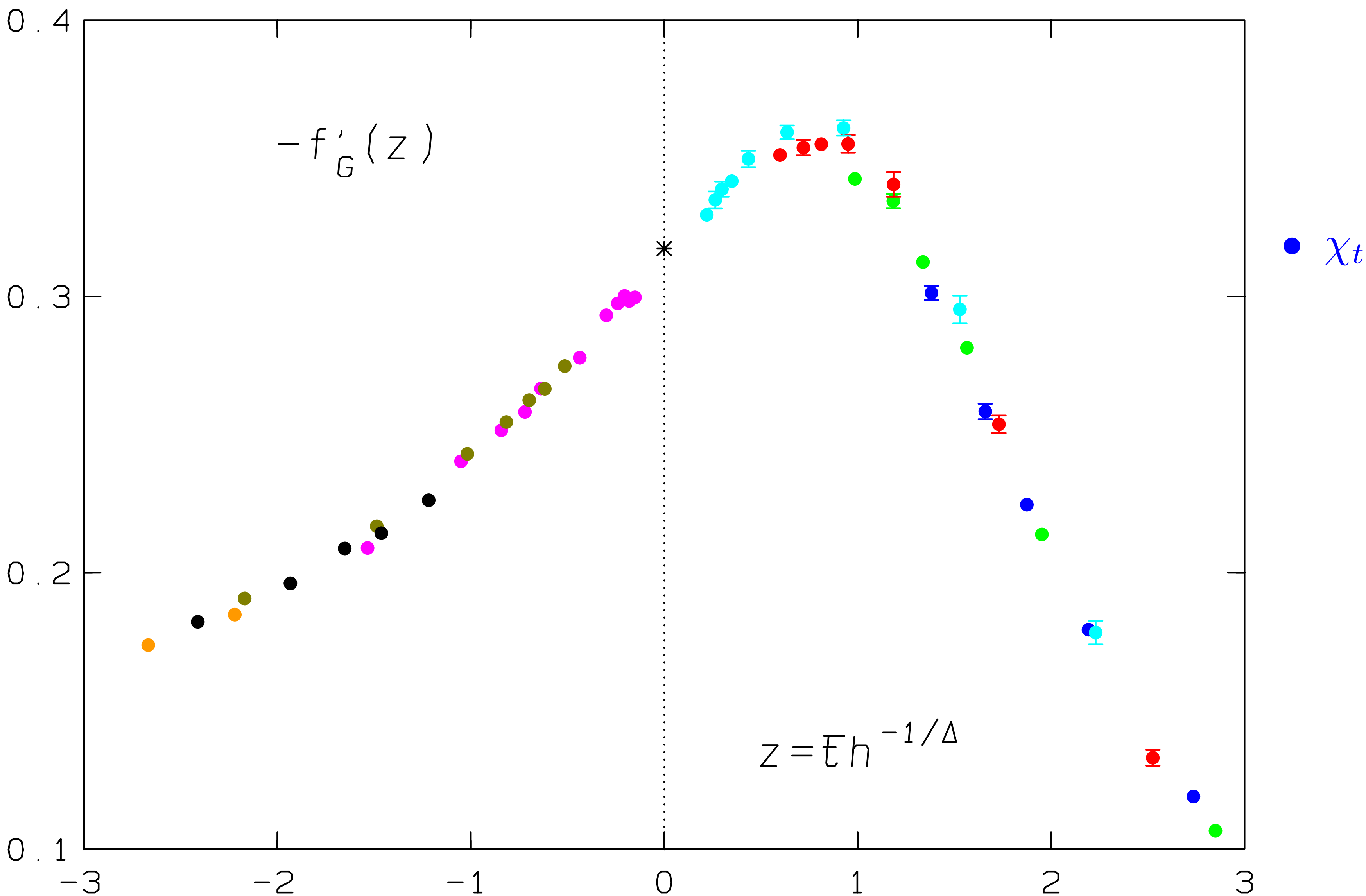
3. Compute leading asymptotic coefficients $c_0^\pm$ of $f_f(z)$.

$\Longrightarrow \quad f'_f(z)$ is parametrized.

Parametrizing the Scaling Function $f_G(z)$



Data for the Scaling Function $-f'_G(z)$



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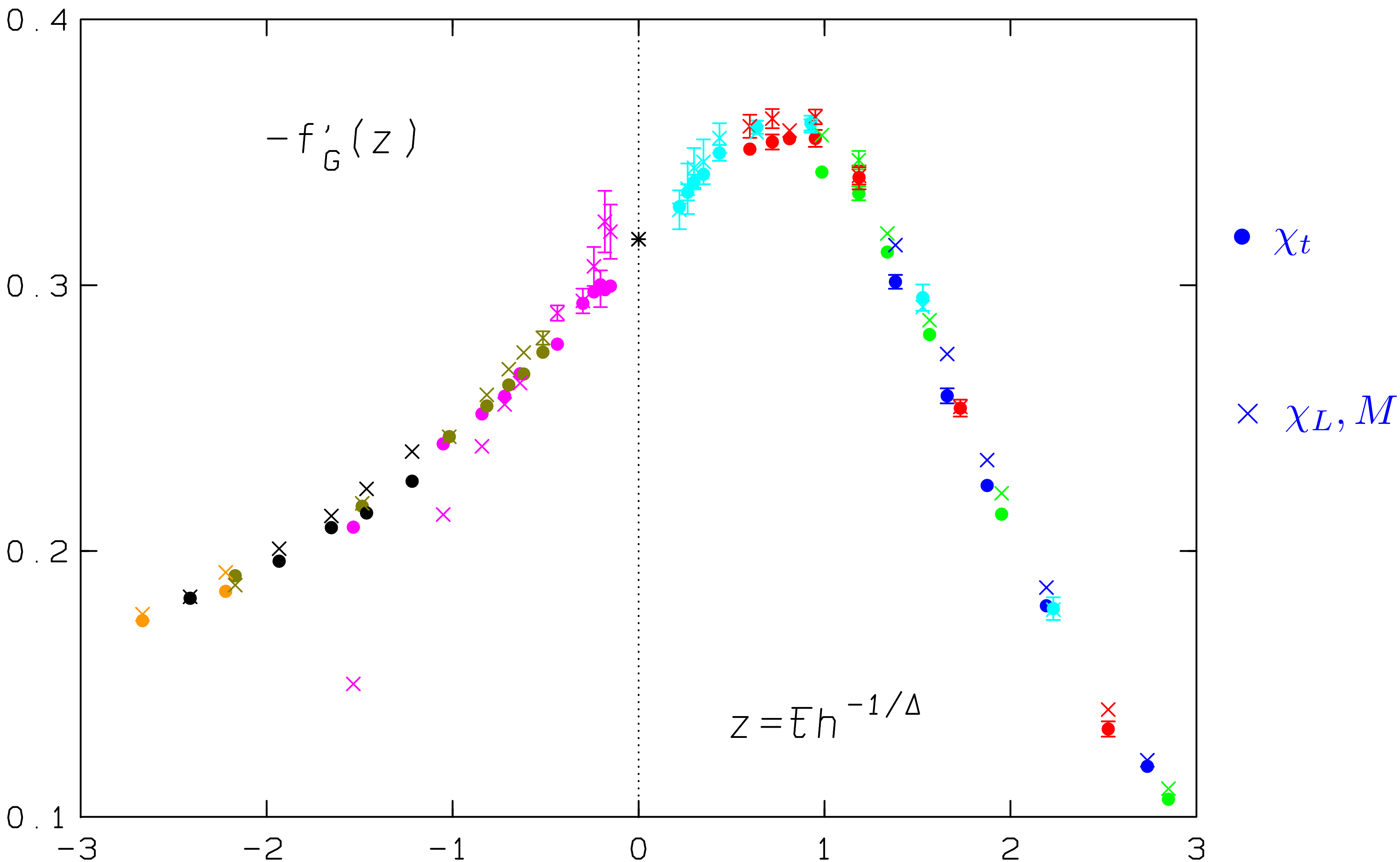

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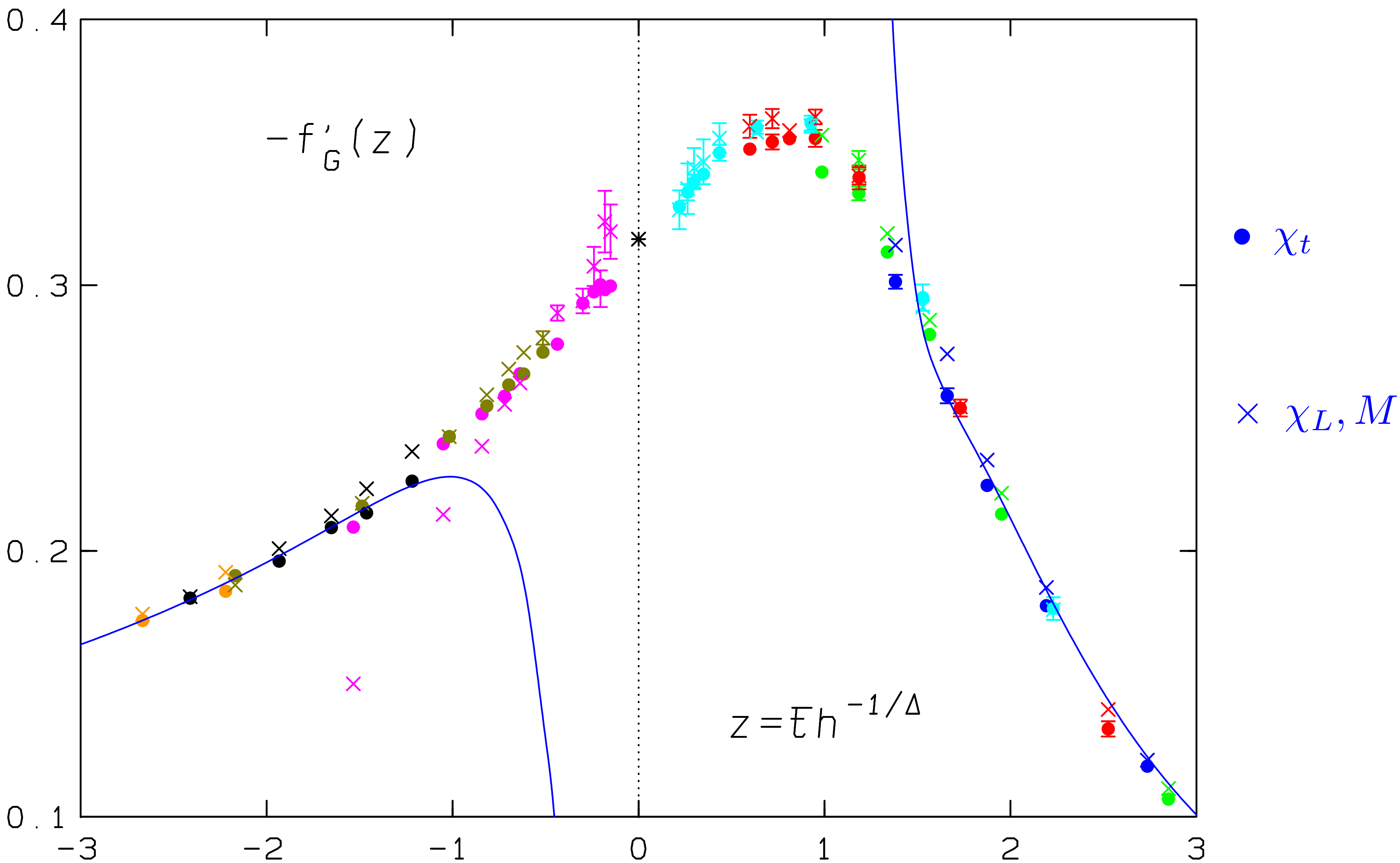

Small z Fit of $-f'_G(z)$

We use only χ_t-data for $z < 1.3$ and for $z \in [1.3, 2]$ both data types.
Then a fit with a truncated small z-series

$$f'_G(z) = b_1 + 2b_2 z + 3b_3 z^2 + 4b_4 z^3 + 5b_5 z^4 + 6b_6 z^5$$

in the overlapping z-intervalls $[-2.5, 0.75]$ and $[-0.75, 2]$ is carried out.

$\Longrightarrow$ average results for b_1 and b_2, fix them and repeat fits; average result for b_3 from 1. and 2. step; fix b_3 and repeat fits; Final result:

b_4^+ and b_4^- coincide inside error bars, $b_5^\pm$, $b_6^\pm$ not.
The fits overlap with the asymptotic fits; we use them in the intervall $[-2, 1.95]$.

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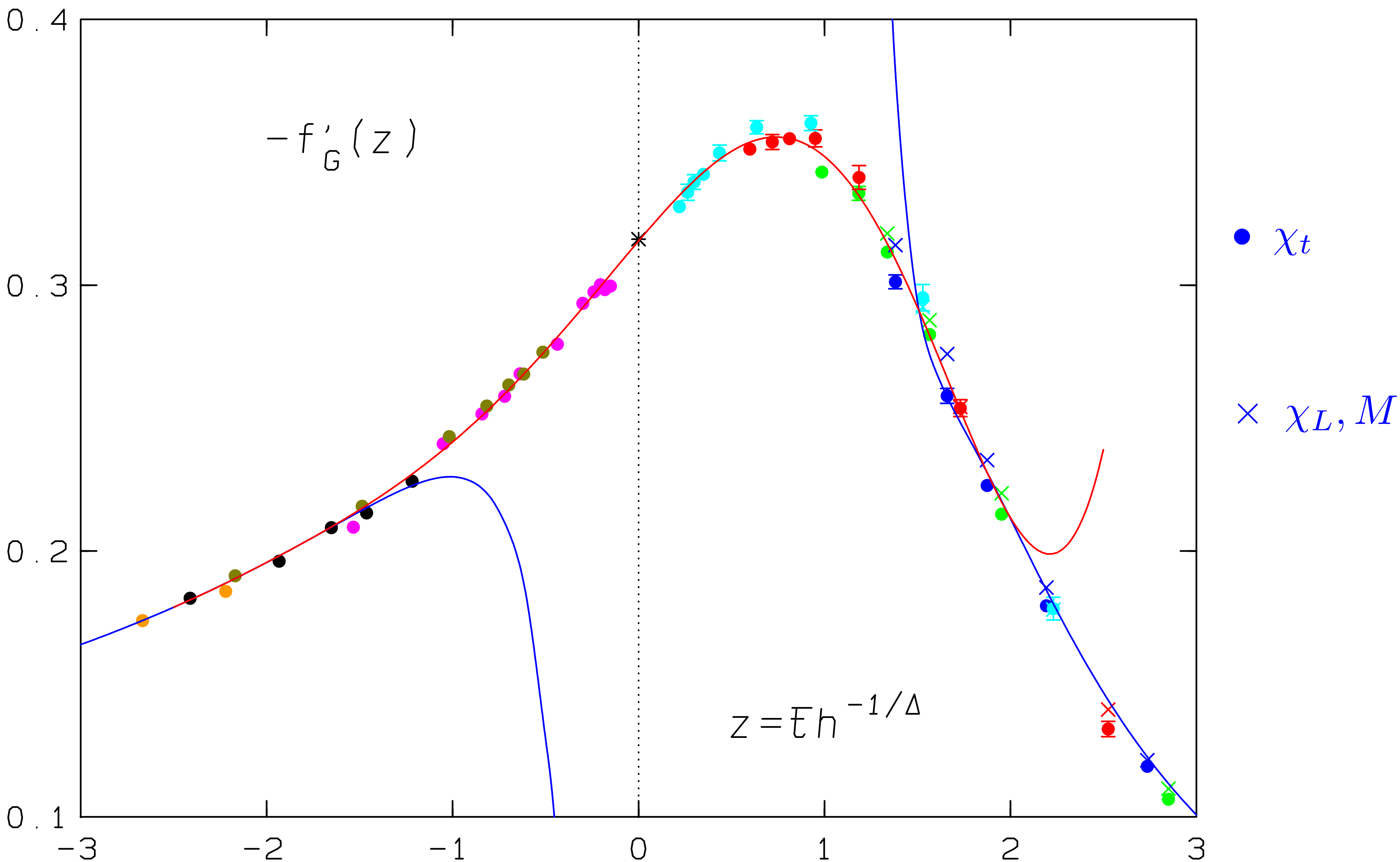
Leading asymptotic coefficients of $f_f(z)$:

$$c_0^+ = 0.42206 \pm 0.01060\ , \quad c_0^- = 0.22918 \pm 0.01067$$

$$\Longrightarrow \quad A^+/A^- = 1.842 \pm 0.043$$

For comparison: Toldin et al. : $1.91(10)$, Cucchieri et al. : $1.8(2)$

Fit of the Scaling Function $-f'_G(z)$



Scaling Tests for ϵ and C, the Non-singular Parts of ϵ and C

$\epsilon(T_c)$ is finite for continuous transitions $\Longrightarrow$ $\alpha < 1$, here $\alpha = -0.213$

$$\hookrightarrow \quad \epsilon_s(T_c, H = 0) = 0 \; , \quad \text{and} \quad \epsilon(T_c, H = 0) = \epsilon_{ns}(T_c)$$

$$\epsilon(T_c, H) = \epsilon_{ns}(T_c) - T_c^2 \frac{H_0}{T_0} h^{(1-\alpha)/\Delta} f_f'(0)$$

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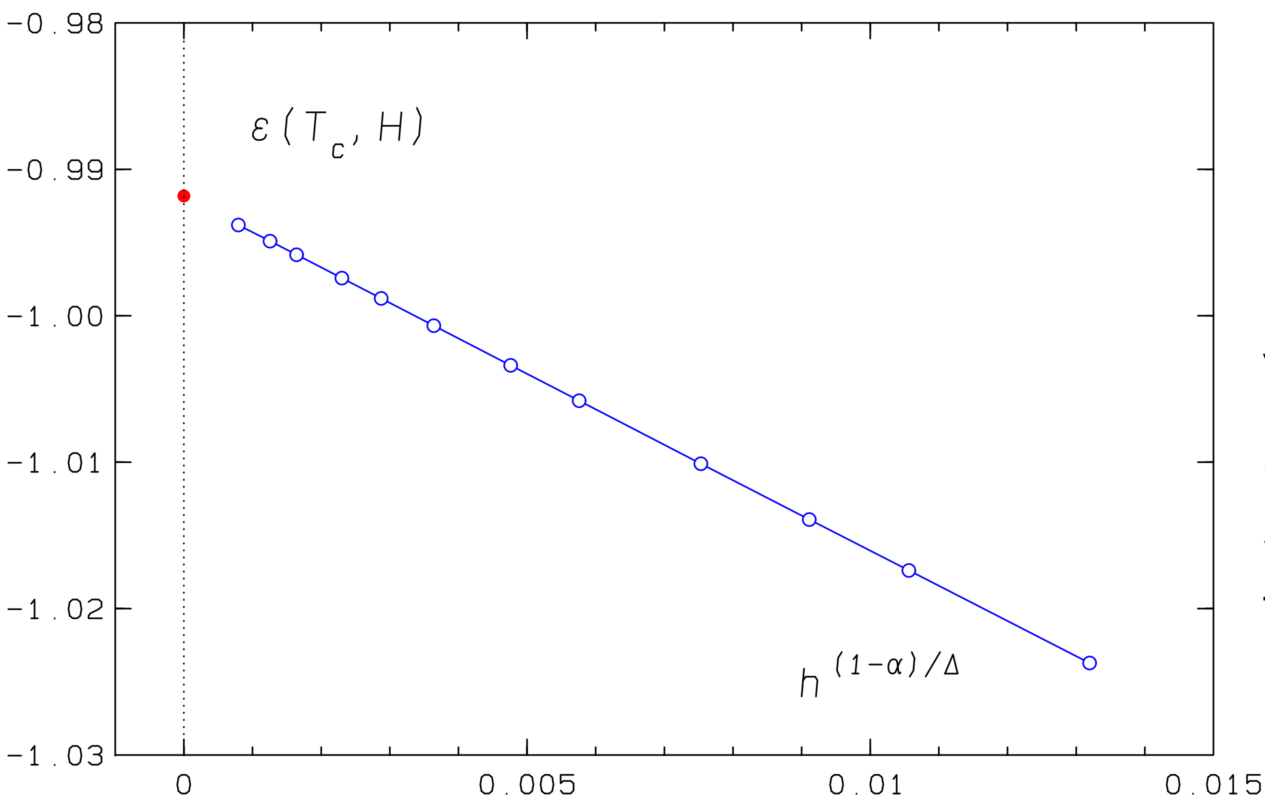

Fit results:

$\epsilon_{ns}(T_c) = -0.991888(13)$

$f_f'(0) = \ 0.47723(32)$

Very accurate! no further H-dependence, no finite size effects! From b_1 one finds $f_f'(0) = \ 0.47843(81)$

Scaling Tests for ϵ and C , the Non-singular Parts of ϵ and C

$C_{ns}(T_c) = ?$ If $\alpha > 0$ $C_s(T, H=0)$ diverges at T_c $\sim |t|^{-\alpha}$

If $\alpha < 0$ $C_s(T_c, H=0) = 0$ and $C_{ns}(T_c)$ remains

and can be determined at T_c from

$$C_s - \frac{2\epsilon_s}{T_c} = -\left(\frac{T_c}{T_0}\right)^2 H_0 h^{-\alpha/\Delta} f_f''(0)$$

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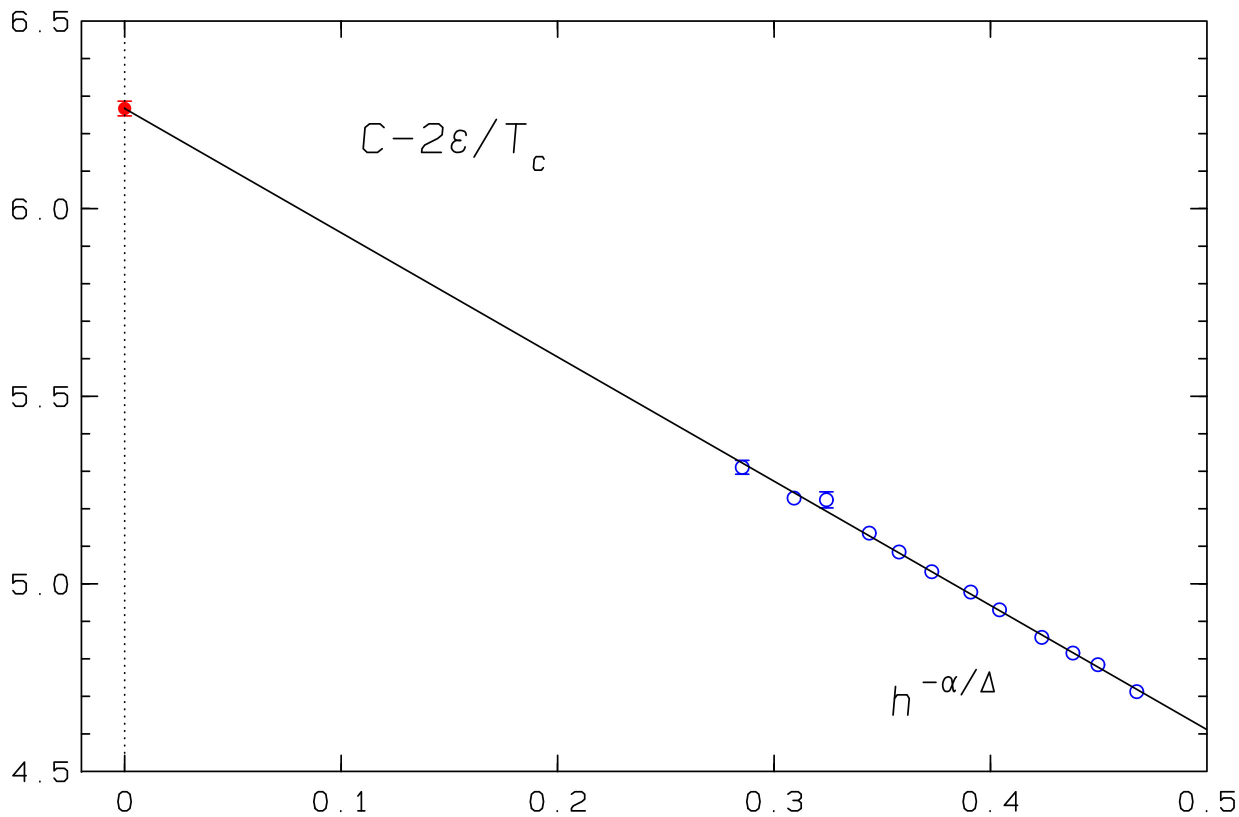


Fit results:

$C_{ns}(T_c) = 4.4103(195)$

$f_f''(0) = 0.7151(104)$

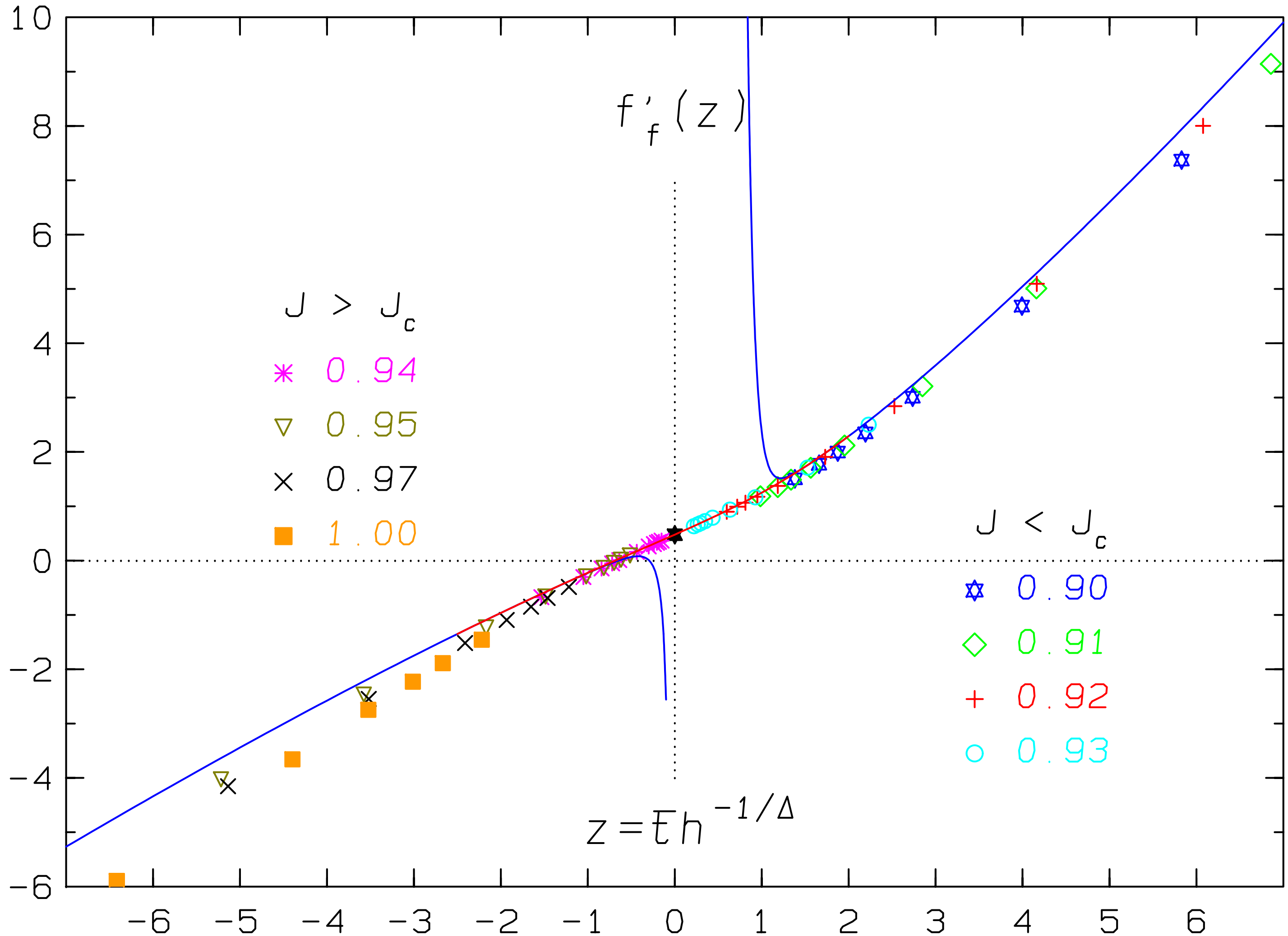
From b_2 one finds

$f_f''(0) = 0.7075(221)$

compatible!

Scaling Test for ϵ, the Function $f'_f(z)$

$$f'_f(z) = -(\epsilon - \epsilon^1_{ns})\frac{T_0}{T^2 H_0} h^{-(1-\alpha)/\Delta}\ , \quad \epsilon^1_{ns}(T) = \epsilon_{ns}(T_c) + (T - T_c)\cdot C_{ns}(T_c)$$



The Non-singular Part of ϵ

Reason for limited scaling: we need a better approximation than $\epsilon^1_{ns}(T)$

Test on H-scaling at fixed T : calculate $\epsilon_{ns}(T)$ from $\epsilon(T, H)$-data and the known scaling function $f'_f(z)$

$$\epsilon_{ns}(T) = \epsilon(T, H) + T^2 \frac{H_0}{T_0} h^{(1-\alpha)/\Delta} f'_f(z)$$

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$$\epsilon_{ns}(T) = \epsilon(T,H) + T^2 \frac{H_0}{T_0} h^{(1-\alpha)/\Delta} f'_f(z)$$

If the test is successful, we must obtain the same value $\epsilon_{ns}(T)$ for all H . This is the case, for example for $J = 0.97 \ (T < T_c) \Longrightarrow$

No corrections to scaling!

The errors of the averages vary for $T < T_c$ between $6 \cdot 10^{-6}$ and $1.4 \cdot 10^{-5}$ and increase to $3.5 \cdot 10^{-5}$ for $T > T_c$.

H	ϵ_{ns}
0.0001	-1.151168(5)
0.0002	-1.151160(3)
0.0005	-1.151159(6)
0.001	-1.151172(5)
0.002	-1.151156(5)
0.003	-1.151150(4)
0.004	-1.151141(5)
0.005	-1.151122(4)
0.007	-1.151103(5)

The Non-singular Part of ϵ

Fit of the found values ($\diamond$) of $\epsilon_{ns}(T)$ with a Taylor expansion up to the third derivative leads to:

$$\epsilon_{ns}(T_c) = -0.991792(28) , \quad C_{ns}(T_c) = 4.3910(14)$$
$$C'_{ns}(T_c) = 8.448(108) , \quad C''_{ns}(T_c) = 42.79 \pm 5.13$$

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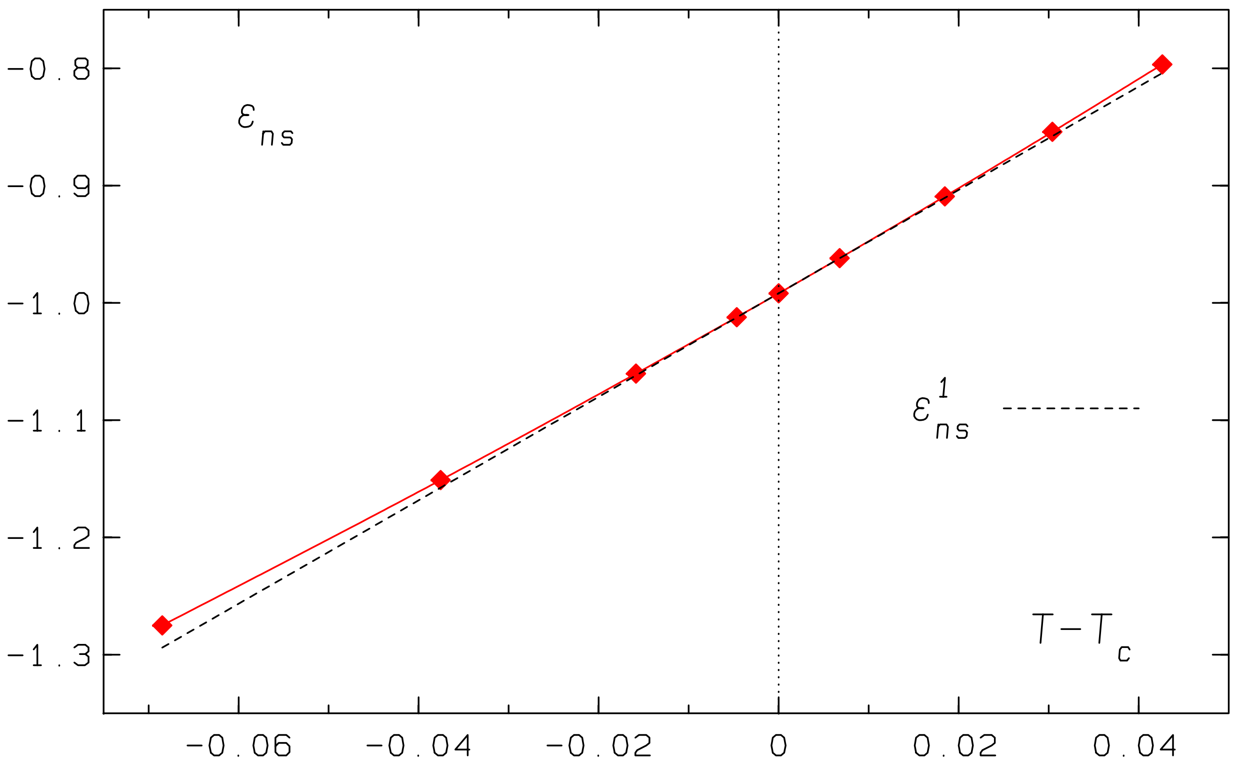
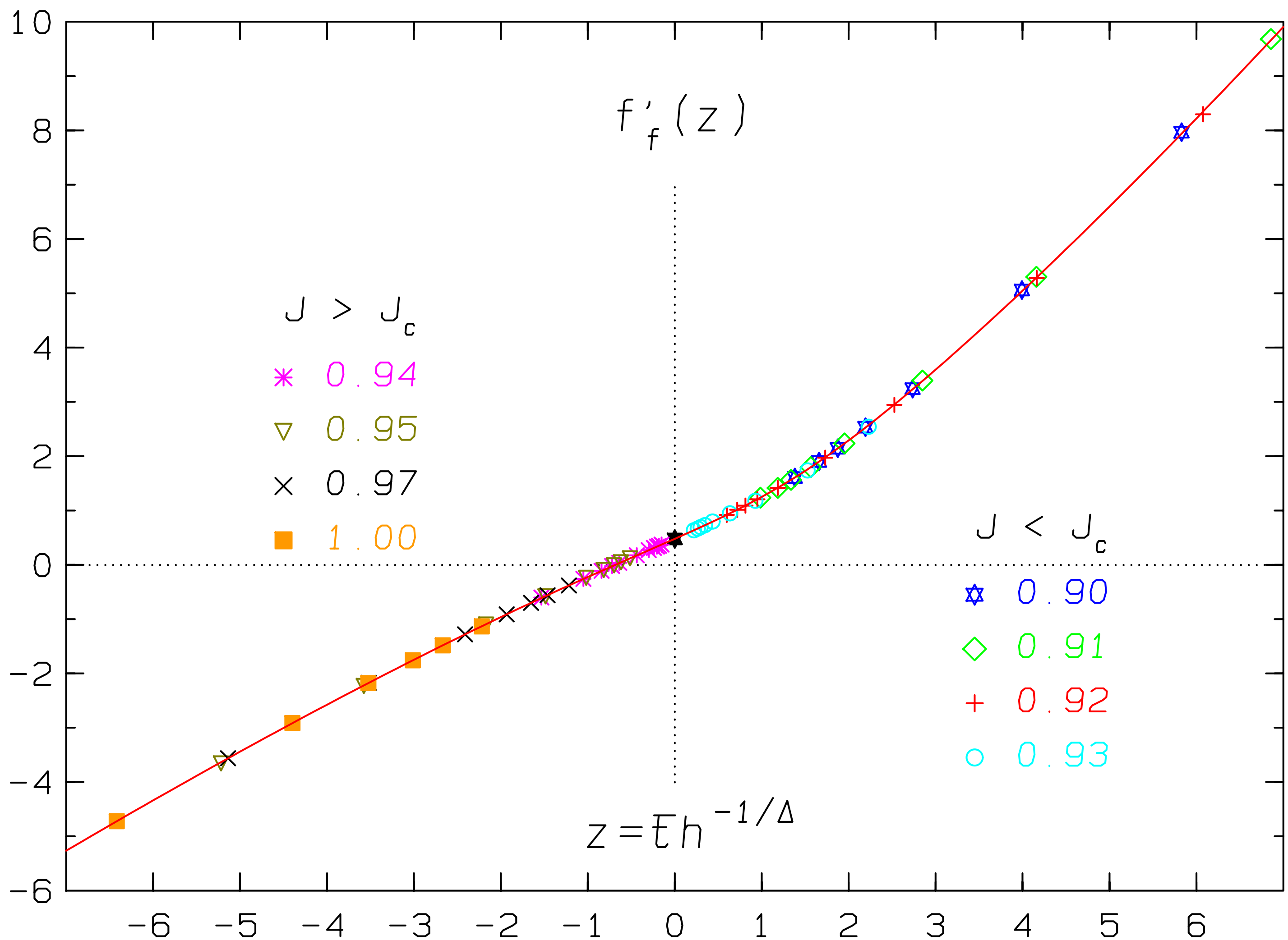


T_c is not a special point of $\epsilon_{ns}(T)$!

$\epsilon_{ns}(T_c)$ and $C_{ns}(T_c)$ are compatible with the results from the direct fits at T_c.

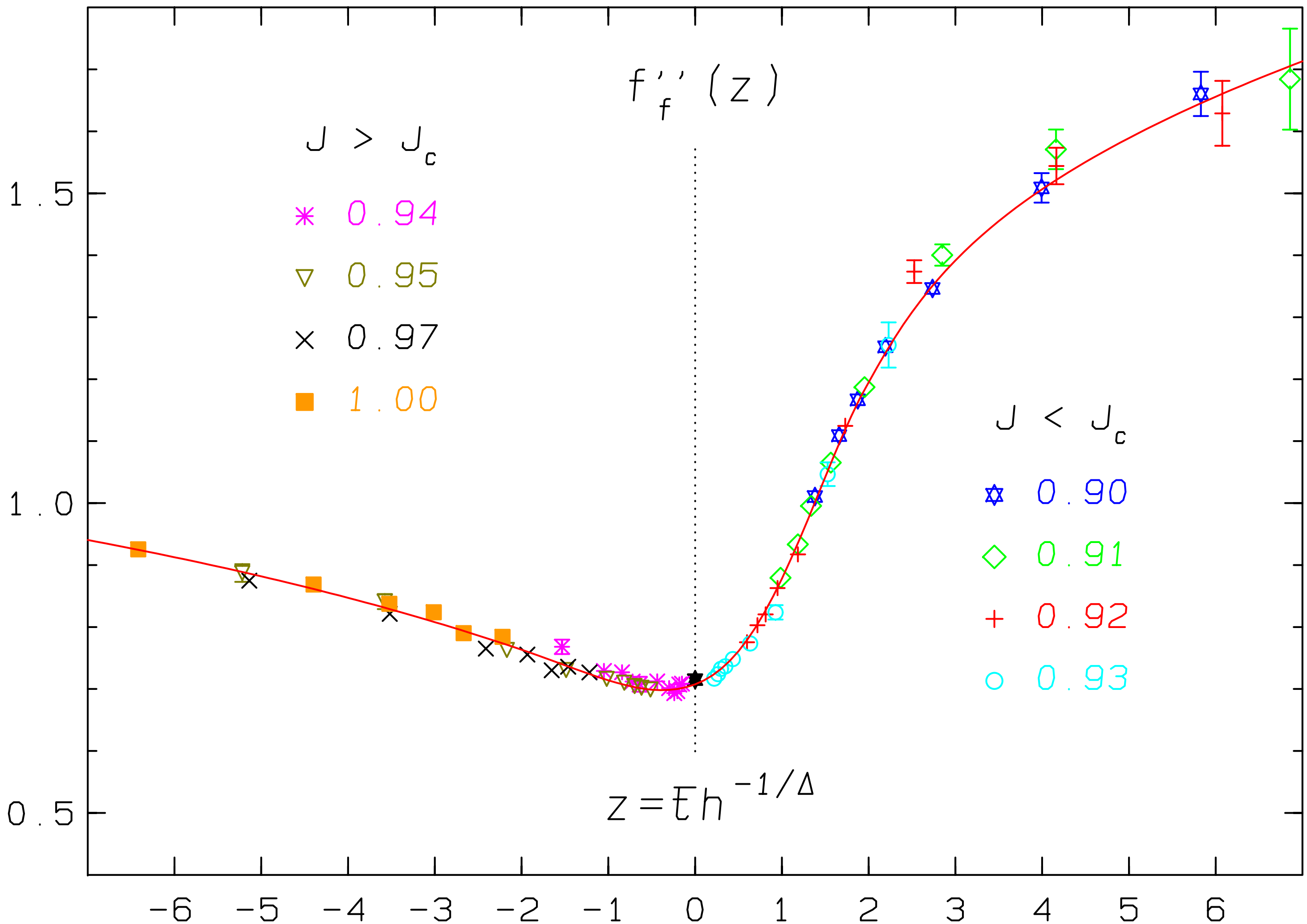
Scaling Test for ϵ, the Function $f_f'(z)$

$$f_f'(z) = -(\epsilon - \epsilon_{ns}^2)\frac{T_0}{T^2 H_0} h^{-(1-\alpha)/\Delta}\ , \quad \epsilon_{ns}^2(T) = \epsilon_{ns}(T_c) + \cdots + \frac{1}{6}(T-T_c)^3 \cdot C_{ns}''(T_c)$$



Scaling Test for C, the Function $f_f''(z)$

$$f_f''(z) = -(C_s - \frac{2}{T}\epsilon_s)\frac{T_0^2}{T^2 H_0} h^{\alpha/\Delta}\,, \quad \epsilon_{ns}^2(T) = \epsilon_{ns}(T_c) + \cdots + \frac{1}{6}(T - T_c)^3 \cdot C_{ns}''(T_c)$$



Summary

We have investigated the scaling functions of the free energy density and its derivatives for the $3d\ O(4)$ model.

In contrast to other papers we have not chosen the historic Widom-Griffiths form for the parametrization of these functions, but a form which is directly derivable from RG theory. Here, the scaling variable z depends only on t and H, not on an observable.

We show that the necessary conditions for a successful parametrization guaranteeing the empirical scaling laws, Griffiths's condition and the inclusion of Goldstone mode effects can be formulated as well for the form we use.

Our parametrization has the advantage that it can be derived directly from data. Correspondingly it is well suited for scaling tests of other models, and these tests can be easily extended to other observables besides the order parameter.

Furthermore we have demonstrated that the critical behaviour of all our data for the $3d\ O(4)$ model is consistently described by the scaling functions we have derived. In addition, we were able to find the non-singular parts of the energy density and the specific heat.

Higher T-derivatives of the Free Energy Density

$$\frac{\partial^n f}{\partial T^n} = \frac{\partial^n f_{ns}}{\partial T^n} + \frac{H_0}{T_0^n} h^{(2-\alpha-n)/\Delta} f_f^{(n)}(z)$$

The 3. derivative is the first one for $\alpha < 0$, which diverges at $T_c \; (z = 0)$ for $H \to 0$

$$\frac{\partial^3 f}{\partial T^3} = \frac{\partial^3 f_{ns}}{\partial T^3} + \frac{H_0}{T_0^3} h^{-(1+\alpha)/\Delta} f_f^{(3)}(z)$$

$\Longrightarrow$ the non-singular term is not as important as before at T_c .

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These higher T-derivatives are of interest in QCD with 2 degenerate light quarks, $m_q = m_u = m_d$ and a small quark chemical potential $\mu_q = \mu_B/3$. Here

$$\bar{t} = \frac{T_c}{T_0}\left(\frac{T-T_c}{T_c} + \kappa_q \left(\frac{\mu_q}{T}\right)^2\right) , \qquad T_c = T_c(\mu_q = 0)$$

$$h = \frac{1}{H_0}\frac{m_q}{T} , \qquad \kappa_q \approx 0.06$$

Higher T-derivatives of the Free Energy Density in QCD

Cumulants of the net baryon number fluctuations

$$\chi_n^B = -\frac{1}{3^n}\frac{\partial^n f}{\partial \hat{\mu}_q^n} \, , \qquad \hat{\mu}_q = \frac{\mu_q}{T}$$

Leading terms near the critical temperature (m_q or $h \to 0$):

$$\chi_n^B \sim \begin{cases} -(2\kappa_q)^{n/2} h^{(2-\alpha-n/2)/\Delta} f_f^{(n/2)} & \text{for} \quad \hat{\mu}_q = 0 \, , \; n \text{ even} \\ -(2\kappa_q)^n \, h^{(2-\alpha-n)/\Delta} \, f_f^{(n)} & \text{for} \quad \hat{\mu}_q > 0 \end{cases}$$

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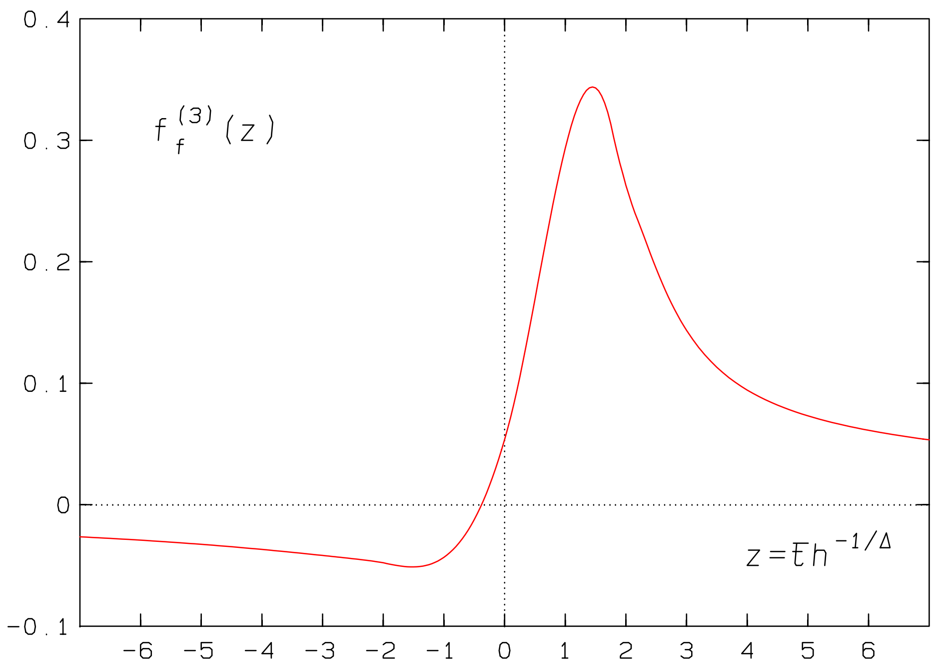

The first diverging cumulant at $\mu_q = 0$ is obtained for $n = 6$ and $\sim f_f^{(3)}(z)$

B. Friman et al. , Eur. Phys. J. C71 (2011) 1694