Exercise on universal scaling fits

Christian Schmidt

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1 Introduction on Scaling Functions

We assume that the free energy (f) can be split into a singular (f_s) and a regular part f_{reg},

$$f(T, H, L) = f_s(T, H, L) + f_{reg}(T, H, L), \tag{1}$$

and that the singular part is given as a generalized homogeneous function of its arguments,

$$f_s(t, h, l) = b^{-d} f_s(b^{y_t} t, b^{y_h} h, bl)\,. \tag{2}$$

Here b is a free scale parameter and y_t and y_h are two relevant critical exponents. We also introduced the relevant scaling fields, the reduced temperature (t), the external symmetry-breaking field (h), and the finite size scaling variable (l), given as

$$t = \frac{1}{t_0}\frac{T - T_c}{T_c}\,, \qquad \frac{H}{H_0}\,, \qquad \frac{L}{L_0}\,. \tag{3}$$

They are normalized by non-universal scale parameters t_0, H_0 and L_0, respectively. The exponents y_t and y_h define the two independent critical exponents of the universality class under consideration,

$$y_t = 1/\nu\,, \qquad y_h = \beta\delta/\nu\,. \tag{4}$$

If we chose $b = h^{-1/y_h}$, we obtain for the free energy

$$f(T, H, L) = H_0 h^{1+1/\delta} f_f(z, z_L) + f_{reg}(T, H, L)\,, \tag{5}$$

where the scaling variables are given as

$$z = t/h^{1/\beta\delta} \qquad \text{and} \qquad z_L = l/h^{\nu/\beta\delta}\,. \tag{6}$$

Finally we obtain for the order parameter $M = -\partial f/\partial H$,

$$M = h^{1/\delta} f_G(z, z_L) + M_{reg}(t, h)\,, \tag{7}$$

with the scaling function

$$f_G(z, z_L) = -\left(1 + \frac{1}{\delta}\right) f_f(z, z_L) + \frac{z}{\beta\delta}\frac{\partial f_f(z, z_L)}{\partial z} + \frac{\nu}{\beta\delta} z_L \frac{\partial f_f(z, z_L)}{\partial z_L}\,. \tag{8}$$

The regular part has the form

$$M_{reg} = a_t t h + b_1 h + \mathcal{O}(h^3)\,. \tag{9}$$

N	h_3	h_5	θ_0	β	δ	Δ
2	0.162(20)	-0.0226(18)	1.610(14)	0.34864(7)	4.7798(5)	1.6664(5)
4	0.306(34)	-0.00338(25)	1.359(10)	0.380(2)	4.824(9)	1.833(13)

Table 1: Parameters of the function $h(\theta)$ and critical exponents for the O(N)-symmetric case.

2 The Schofield Parametrization

The scaling function obtained in analytic calculations are commonly parameterized using the Schofield parametrization [1]. In this paramtrization the alternative scaling variable θ is used. In the infinite volume ($z_L = 0$), a relation between θ and and the scaling function $f_G(z) \equiv f_G(z, 0)$ in the Widom-Griffiths form [2] and the scaling variable z can be made,

$$f_G(z) \equiv f_G(\theta(z)) = \theta \left(\frac{h(\theta)}{h(1)} \right)^{-1/\delta} , \tag{10}$$

$$z(\theta) = \frac{1-\theta^2}{\theta_0^2 - 1} \theta_0^{1/\beta} \left(\frac{h(\theta)}{h(1)} \right)^{-1/\beta\delta} . \tag{11}$$

The auxiliary function $h(\theta)$ is given in the form

$$h(\theta) = (\theta + h_3\theta^3 + h_5\theta^5)(1 - \theta^2/\theta_0^2)^2 . \tag{12}$$

The parameters h_3, h_5 and θ_0 have been determined in Monte Carlo Simulations [3], [4]. Values for the O(N) symmetric case, with $N = 2, 4$ are given in Table 1. Also Given in Table 1 are values for the critical exponents β, δ, and $\Delta = \beta\delta$, taken from [5], [6].

3 Exercises

Here we apply some scaling fits to data, which was obtained by lattice QCD calculations of (2+1)-flavor QCD for smaller than physical pion masses [7].

1. Look at the file *ChiralData.py*, which defines a class to read and access the data for various lattice sizes (volumes and lattice spacings), masses and temperatures. If you call the python file, you should crate two pictures with all the available data, one for the chiral condensate and one for the chiral susceptibility.

2. Now consider the file *ChiralFunc.py*. Here you should implement the functions $\theta(z)$, $f_G(\theta)$ from Sec. 2. What is the relevant interval $\theta \in [a, b]$, in order to create z-values from $(-\infty, +\infty)$? You also need to numerically invert the function $z(\theta)$ to obtain $\theta(z)$. Hint: use the bisection method from *scipy.optimize* with the starting interval $[a + \epsilon, b - \epsilon]$. When you call the file *ChiralFunc.py* you should generate two pictures, one showing $z(\theta)$

and one $f_G(\theta(z))$. Generate two sets of data for both pictures, one with equidistant points in θ and one with equidistant points in z.

3. Use the optimizer from SciPy to perform a infinite size O(4) scaling fit to the order parameter (chiral condensate) for the $N_\tau = 8$ lattices. A skeleton is given in *ChiralFit.py*. You have to implement the magnetic equation of state (Eq. (7)) as the actual fitting function. As fit parameter use T_c (chiral transition temperature), $z_0 \equiv h_0^{1/\beta\delta}/t_0$ and h_0. Start with only including the smallest two quark masses, and temperatures in the interval $T \in [T_{center} - T_{delta}, T_{center} + T_{delta}]$, where $T_{center} = 144$ MeV and T_{delta}=14 MeV. If this fit is working, you can successively include larger masses. Note that for higher masses you might need to include a regular term. You should create two plots, one which shows the chiral condensate as function of T for different masses and one which shows the data collapse, i.e. $h^\delta M$ as function of z.

   If you still have time, you can try to

   - investigate differences between the O(2) and O(4) scaling functions, by choosing the appropriate parameters from Table 1.
   - implement the scaling function f_χ, given as

     $$f_\chi(z, z_L) = \frac{1}{\delta}\left(f_G(z, z_L) - \frac{z}{\beta} f_G'(z, z_L)\right) - \frac{\nu}{\beta\delta} z_L \frac{\partial f_f(z, z_L)}{\partial z_L} \,. \quad (13)$$

     With f_χ you can predict the chiral susceptibility from your scaling fit to f_G, we have

     $$\chi_h(T, H, L) = H_0^{-1} h^{1/\delta - 1} f_\chi(z, z_L) + \chi_{h,reg} \,. \quad (14)$$

     You can also perform a separate scaling fit to the chiral susceptibility.
   - implement finite size corrections. These correction will be most relevant for the scaling fit to f_χ. The corrections have been parametrized in [4] in the form

     $$f_G(z, z_L) = f_G(z, 0) + \sum_{n=1}^{n_u} \sum_{m=3}^{m_u} a_{nm} z^n z_L^m \,, \quad (15)$$

     $$f_\chi(z, z_L) = f_\chi(z, 0) + \sum_{n=1}^{n_u} \sum_{m=3}^{m_u} \left(\frac{1}{\delta} - \frac{n + m\nu}{\beta\delta}\right) a_{nm} z^n z_L^m \,. \quad (16)$$

     The parameters a_{nm} can be taken from Table I of [3] for O(4) and Table VIII of [4] for O(2).

References

[1] P. Schofield, "Parametric Representation of the Equation of State Near A Critical Point," *Phys. Rev. Lett.*, vol. 22, pp. 606–608, 1969. DOI: 10.1103/PhysRevLett.22.606.

[2] R. B. Griffiths, “Thermodynamic Functions for Fluids and Ferromagnets near the Critical Point,” *Phys. Rev.*, vol. 158, pp. 176–187, 1967. DOI: 10.1103/PhysRev.158.176.

[3] J. Engels and F. Karsch, “The scaling functions of the free energy density and its derivatives for the 3d O(4) model,” *Phys. Rev. D*, vol. 85, p. 094 506, 2012. DOI: 10.1103/PhysRevD.85.094506. arXiv: 1105.0584 [hep-lat].

[4] F. Karsch, M. Neumann, and M. Sarkar, “Scaling functions of the three-dimensional Z(2), O(2), and O(4) models and their finite-size dependence in an external field,” *Phys. Rev. D*, vol. 108, no. 1, p. 014 505, 2023. DOI: 10.1103/PhysRevD.108.014505. arXiv: 2304.01710 [hep-lat].

[5] M. Hasenbusch, “Monte Carlo study of an improved clock model in three dimensions,” *Phys. Rev. B*, vol. 100, no. 22, p. 224 517, 2019. DOI: 10.1103/PhysRevB.100.224517. arXiv: 1910.05916 [cond-mat.stat-mech].

[6] J. Engels, L. Fromme, and M. Seniuch, “Correlation lengths and scaling functions in the three-dimensional O(4) model,” *Nucl. Phys. B*, vol. 675, pp. 533–554, 2003. DOI: 10.1016/j.nuclphysb.2003.09.060. arXiv: hep-lat/0307032.

[7] H. T. Ding *et al.*, “Chiral Phase Transition Temperature in (2+1)-Flavor QCD,” *Phys. Rev. Lett.*, vol. 123, no. 6, p. 062 002, 2019. DOI: 10.1103/PhysRevLett.123.062002. arXiv: 1903.04801 [hep-lat].