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Critical equation of state from the average action

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Abstract

The scaling form of the critical equation of state is computed for $O(N)$-symmetric models. We employ a method based on an exact flow equation for a coarse grained free energy. A suitable truncation is solved numerically.

A precise computation of the critical equation of state near a second order phase transition is an old problem. From a general renormalisation group analysis [1] one can prove the Widom scaling form [2] $H = \phi^\delta \tilde{f}((T-T_c)/\phi^{1/\beta})$ for the relation between the magnetic field H, the magnetisation ϕ and the difference from the critical temperature $T-T_c$. In several models the critical exponents β and δ have been computed with high accuracy [3] but the scaling function $\tilde{f}$ is more difficult to access. Previous attempts include an expansion in $4-\epsilon$ dimensions in second order in ϵ (third order for the Ising model) [3]. A particular difficulty for a direct computation in three dimensions arises from the existence of massless Goldstone modes in the phase with spontaneous symmetry breaking for models with continuous symmetry (e.g. Heisenberg models with $O(N)$ symmetry for $N>1$). They introduce severe infrared problems within perturbative or loop expansions.

Recently a non-perturbative method has been proposed which can systematically deal with infrared problems. It is based on the average action Γ_k [4] which is a coarse grained free energy with an infrared cutoff. More precisely Γ_k includes the effects of all fluctuations with momenta $q^2 > k^2$ but not those with $q^2 < k^2$. In the limit $k \to 0$ the average action becomes the standard effective action (the generating functional of the 1PI Green functions), while for $k \to \infty$ it equals the classical or microscopic action. It is formulated in continuous space and all symmetries of the model are preserved. There is a simple functional integral representation [4] of Γ_k also for $k > 0$ such that its couplings can, in principle, also be estimated by alternative methods.

The exact non-perturbative flow equation [5] for the scale dependence of Γ_k takes the simple form of a renormalisation group improved one-loop equation [4]

$$k\frac{\partial}{\partial k}\Gamma_k[\phi] = \frac{1}{2}\mathrm{Tr}\left[\left(\Gamma_k^{(2)}[\phi] + R_k\right)^{-1} k\frac{\partial}{\partial k}R_k\right]. \tag{1}$$

The trace involves a momentum integration and summation over internal indices. Most importantly, the relevant infrared properties appear directly in the form of the exact inverse average propagator $\Gamma_k^{(2)}$, which is the matrix of second functional derivatives with respect to the fields. There is always only one momentum integration - multi-loops are not needed - which is, for a suitable cutoff function $R_k(q^2)$ (with $R_k(0) \sim k^2$, $R_k(q^2 \to \infty) \sim e^{-q^2/k^2}$), both infrared and ultraviolet finite.

The flow equation (1) is a functional differential equation and an approximate solution requires a truncation. Our truncation is the lowest order in a systematic derivative expansion of Γ_k [4, 6, 7]

$$\Gamma_k = \int d^d x \left\{ U_k(\rho) + \frac{1}{2} Z_k \partial^\mu \phi_a \partial_\mu \phi^a \right\}. \tag{2}$$

Here ϕ^a denotes the N-component real scalar field and $\rho = \frac{1}{2}\phi^a\phi_a$. We keep for the potential term the most general $O(N)$-symmetric form $U_k(\rho)$ since $U_0(\rho)$ encodes the equation of state. The wavefunction renormalisation is approximated by one k-dependent parameter Z_k. Next order in the derivative expansion would be the generalization to a ρ-dependent wavefunction renormalisation $Z_k(\rho)$ plus a function $Y_k(\rho)$ accounting for a possible different index structure of the kinetic term for $N \geq 2$ [4, 6]. Going further would require the consideration of terms with four derivatives and so on. Concerning the equation of state for the present model, the omission of higher derivative terms in the average action typically generates an uncertainty of the order of the anomalous dimension η. The main reason is that for $\eta = 0$ the kinetic term in the k-dependent inverse propagator must be exactly proportional to q^2 both for $q^2 \to 0$ and $q^2 \to \infty$. For the three-dimensional scalar theory η is known to be small and the derivative expansion is, therefore, expected to give a reliable approximation. This holds for arbitrary constant "background" field ϕ^a. Similar, although less stringent, arguments indicate a weak ρ-dependence of the kinetic term. For the scaling solution for $N = 1$ this weak ρ-dependence has been established explicitly [7].

In this letter we compute the effective potential (Helmholtz free energy) $\lim_{k\to 0} U_k(\rho) \equiv U(\rho)$ for the $O(N)$-model directly in three dimensions from a solution of eqs. (1), (2). We extract the Widom scaling form of the equation of state and give semi-analytical expressions for $N = 1$ and $N = 3$. Its asymptotic behavior yields the universal critical exponents and amplitude ratios. An alternative parametrisation of the equation of state in terms of renormalised quantities is used in order to compute universal couplings.

For a study of the behavior in the vicinity of the phase transition it is convenient to work with dimensionless renormalised fields

$$\tilde{\rho} = Z_k k^{-1} \rho, \qquad u_k(\tilde{\rho}) = k^{-3} U_k(\rho(\tilde{\rho})). \tag{3}$$

With the truncation of eq. (2) the exact evolution equation for $u'_k \equiv \partial u_k / \partial \tilde{\rho}$ [4, 6] reduces to the partial differential equation

$$\begin{aligned} \frac{\partial u'_k}{\partial t} &= \Big(-2+\eta\Big) u'_k + \Big(1+\eta\Big)\tilde{\rho} u''_k \\ &\quad - \frac{(N-1)}{4\pi^2} u''_k l_1^3\Big(u'_k;\eta\Big) - \frac{1}{4\pi^2}\Big(3u''_k + 2\tilde{\rho}u'''_k\Big) l_1^3\Big(u'_k + 2\tilde{\rho}u''_k;\eta\Big), \end{aligned} \tag{4}$$

where $t = \ln(k/\Lambda)$, with Λ the ultraviolet cutoff of the theory. The anomalous dimension η is given in our truncation by [4, 6]

$$\eta = -\frac{\partial}{\partial t} \ln Z_k = \frac{2}{3\pi^2} \kappa \lambda^2 m_{2,2}^3(2\lambda\kappa). \tag{5}$$

with κ the location of the minimum of the potential, $u'_k(\kappa) = 0$, and λ the quartic coupling, $u''_k(\kappa) = \lambda$. The "threshold" functions l_1^3 and $m_{2,2}^3$ result from the momentum integration on the r.h.s. of eq. (1) and account for the decoupling of modes with effective mass larger than k. They equal constants of order one for vanishing arguments and decay fast for arguments much larger than one. For the choice of the cutoff function R_k employed here their explicit form can be found in refs. [6, 8].

To obtain the equation of state one has to solve the partial differential equation (4) for $k \to 0$. Algorithms adapted to the numerical solution of eq. (4) have been developed previously [8] and we refer to this work for details. The integration starts at some short distance scale $k^{-1} = \Lambda^{-1}$ $(t = 0)$ where the average potential is equal to the microscopic or classical potential (no integration of fluctuations has been performed). We start with a quartic classical potential parametrized as $u'_\Lambda(\tilde{\rho}) = \lambda_\Lambda(\tilde{\rho} - \kappa_\Lambda)$. In the phase with spontaneous symmetry breaking the order parameter $\rho_0 = \lim_{k\to 0} Z_k^{-1} k\kappa$ takes a non-vanishing value. In the symmetric phase the order parameter vanishes, i.e. $\rho_0 = 0$ for $k = 0$. The two phases are separated by a scaling solution for which $u'_k(\tilde{\rho})$ becomes independent of k. For any given λ_Λ there is a critical value κ_{cr} for which the evolution leads to the scaling solution. A measure of the distance from the phase transition is the difference $\delta\kappa_\Lambda = \kappa_\Lambda - \kappa_{cr}$. If κ_Λ is interpreted as a function of temperature, the deviation $\delta\kappa_\Lambda$ is proportional to the deviation from the critical temperature, i.e. $\delta\kappa_\Lambda = A(T)(T_c - T)$ with $A(T_c) > 0$.

The external field H is related to the derivative of the effective potential $U' = \partial U/\partial\rho$ by $H_a = U'\phi_a$. The critical equation of state relating the temperature, the external field and the order parameter can then be written in the scaling form ($\phi = \sqrt{2\rho}$)

$$\frac{U'}{\phi^{\delta-1}} = f(x), \qquad x = \frac{-\delta\kappa_\Lambda}{\phi^{1/\beta}} \tag{6}$$

with critical exponents δ and β. For $\phi \to \infty$ our numerical solution for U' obeys $U' \sim \phi^{\delta-1}$ to high accuracy. The inferred value of δ is displayed in the table, and we have checked the scaling relation $\delta = (5-\eta)/(1+\eta)$. The value of the critical exponent η is obtained from eq. (5) for the scaling solution [6]. We have also verified explicitly that f depends only on the scaling variable x for the value of β given in the table. In figs. 1 and 2 we plot $\log(f)$ and $\log(df/dx)$ as a function of $\log|x|$ for $N = 1$ and $N = 3$. Fig. 1 corresponds to the symmetric phase ($x > 0$) and fig. 2 to the phase with spontaneous symmetry breaking ($x < 0$).

One can easily extract the asymptotic behavior from the logarithmic plots. The curves become constant both for $x \to 0^+$ and $x \to 0^-$ with the same value, consistently with the regularity of $f(x)$ at $x = 0$. For the universal function one obtains

$$\lim_{x\to 0} f(x) = D \tag{7}$$

and $H = D\phi^\delta$ on the critical isotherm. For $x \to \infty$ one observes that $\log(f)$ becomes a linear function of $\log(x)$ with constant slope γ. In this limit the universal function takes the form

$$\lim_{x\to\infty} f(x) = (C^+)^{-1} x^\gamma, \tag{8}$$

or $\lim_{\phi\to 0} U' = (C^+)^{-1}|\delta\kappa_\Lambda|^\gamma \phi^{\delta-1-\gamma/\beta} = \bar{m}^2$, and we have verified the scaling relation $\gamma/\beta = \delta - 1$. One observes that the zero-field magnetic susceptibility, or equivalently the inverse unrenormalised squared mass $\bar{m}^{-2} = \chi$, is non-analytic for $\delta\kappa_\Lambda \to 0$ in the symmetric phase: $\chi = C^+|\delta\kappa_\Lambda|^{-\gamma}$. In this phase the correlation length $\xi = (Z_0\chi)^{1/2}$, which is equal to the inverse of the renormalised mass m_R, behaves as $\xi = \xi^+|\delta\kappa_\Lambda|^{-\nu}$ with $\nu = \gamma/(2-\eta)$.

In the phase with spontaneous symmetry breaking ($x < 0$) the plot of $\log(f)$ fig. 2 shows a singularity for $x = -B^{-1/\beta}$, i.e.

$$f(x = -B^{-1/\beta}) = 0. \tag{9}$$

The order parameter for $H = 0$ therefore behaves as $\phi = B(\delta\kappa_\Lambda)^\beta$. Below the critical temperature the longitudinal and transversal magnetic susceptibilities χ_L and χ_T are different for $N > 1$ ($f' = df/dx$)

$$\chi_L^{-1} = \frac{\partial^2 U}{\partial\phi^2} = \phi^{\delta-1}\Big(\delta f(x) - \frac{x}{\beta} f'(x)\Big), \qquad \chi_T^{-1} = \frac{1}{\phi}\frac{\partial U}{\partial\phi} = \phi^{\delta-1} f(x). \tag{10}$$

This is related to the existence of massless Goldstone modes in the $(N-1)$ transverse directions which imply that the transversal susceptibility diverges for vanishing external field. Fluctuations of these massless modes also induce a divergence of the zero-field longitudinal susceptibility. This can be seen from the singularity of the plot of $\log(f')$ for $N=3$ in fig. 2. The first derivative of the universal function with respect to x vanishes as $H \to 0$, i.e. $f'(x = -B^{-1/\beta}) = 0$ for $N \geq 2$. For $N=1$ there is a non-vanishing constant value for $f'(x = -B^{-1/\beta})$ with a finite zero-field susceptibility $\chi = C^{-}(\delta\kappa_\Lambda)^{-\gamma}$ where $(C^{-})^{-1} = B^{\delta-1-1/\beta} f'(-B^{-1/\beta})/\beta$. For a non-vanishing physical infrared cutoff k the longitudinal susceptibility remains finite also for $N \geq 2$: $\chi_L \sim (k\rho_0)^{-1/2}$. In the ordered phase the correlation length for $N=1$ behaves as $\xi = \xi^{-}(\delta\kappa_\Lambda)^{-\nu}$ and, also for $N>1$, the renormalised minimum $\rho_{0R} = Z_0\rho_0$ of the potential U scales as $\rho_{0R} = E(\delta\kappa_\Lambda)^{\nu}$.

The amplitudes of singularities near the phase transition D, $C^{\pm}$, $\xi^{\pm}$, B and E are shown in the table. They are not universal since different short distance physics will result in different wavefunction renormalisations Z_φ and Z_{φ^2}. All models in the same universality class can, however, be related by a multiplicative rescaling of ϕ and $\delta\kappa_\Lambda$ (or $T_c - T$) resulting in $x \to c_x x$ and $f \to c_f f$. Ratios of amplitudes which are invariant under this rescaling are universal. We display the universal combinations C^+/C^-, ξ^+/ξ^-, $R_\chi = C^+ D B^{\delta-1}$, $\tilde{R}_\xi = (\xi^+)^{\beta/\nu} D^{1/(\delta+1)} B$ and $\xi^+ E$ in the table.

The asymptotic behavior observed for the universal function can be used to obtain a semi-analytical expression for $f(x)$. We find the following fit to reproduce the numerical values for both f and df/dx within 1% deviation (apart from the immediate vicinity of the zero of f for $N=3$, cf. eq. (17)):

$$f_{fit}(x) = D\Big(1 + B^{1/\beta}x\Big)^{a}\Big(1+\Theta x\Big)^{\Delta}\Big(1+cx\Big)^{\gamma-a-\Delta}, \tag{11}$$

with $c = (C^+ D B^{a/\beta}\Theta^{\Delta})^{-1/(\gamma-a-\Delta)}$. The parameter a is determined by the order of the pole of f^{-1} at $x = -B^{-1/\beta}$, i.e. $a=1$ ($a=2$) for $N=1$ ($N>1$). The fitting parameters are chosen as $\Theta = 0.569$ (1.312) and $\Delta = 0.180$ (-0.595) for $N=1$ (3).

There is an alternative parametrisation of the equation of state in terms of renormalised quantities. In the symmetric phase ($\delta\kappa_\Lambda < 0$) we consider the dimensionless quantity

$$F(s) = \frac{U_R'}{m_R^2} = C^+ x^{-\gamma} f(x), \qquad s = \frac{\rho_R}{m_R} = \frac{1}{2}(\xi^+)^3 (C^+)^{-1} x^{-2\beta} \tag{12}$$

with $\rho_R = Z_0\rho$ and $U_R^{(n)} = Z_0^{-n} U^{(n)}$. The derivatives of F at $s=0$ yield the universal couplings

$$\frac{dF}{ds}(0) = \frac{U_R''(0)}{m_R} \equiv \frac{\lambda_R}{m_R}, \qquad \frac{d^2F}{ds^2}(0) = U_R'''(0) \equiv \nu_R \tag{13}$$

and similarly for higher derivatives. They determine the behavior of f for $x \gg 1/2$

$$f(x) = (C^+)^{-1}x^{\gamma} + \frac{1}{2}\frac{\lambda_R}{m_R}(\xi^+)^3 (C^+)^{-2} x^{\gamma-2\beta} + \frac{1}{8}\nu_R (\xi^+)^6 (C^+)^{-3} x^{\gamma-4\beta} + \ldots \tag{14}$$

In the ordered phase ($\delta\kappa_\Lambda > 0$) we consider the ratio

$$G(\tilde{s}) = \frac{U_R'}{\rho_{0R}^2} = \frac{1}{2}B^2 E^{-3}(-x)^{-\gamma} f(x), \qquad \tilde{s} = \frac{\rho_R}{\rho_{0R}} = B^{-2}(-x)^{-2\beta}. \tag{15}$$

The values for the universal couplings

$$\frac{dG}{d\tilde{s}}(1) = \frac{U_R''(\rho_{0R})}{\rho_{0R}} \equiv \frac{\hat{\lambda}_R}{\rho_{0R}}, \qquad \frac{d^2G}{d\tilde{s}^2}(1) = U_R'''(\rho_{0R}) \equiv \hat{\nu}_R \tag{16}$$

as well as λ_R/m_R and ν_R are given in the table. One observes that for $N > 1$ the renormalised quartic coupling $\hat{\lambda}_R$ vanishes in the ordered phase. This results from the presence of massless fluctuations. For x near $-B^{-1/\beta}$ the scaling function is approximated by

$$f(x) = E^3 B^{-6}(-x)^\gamma \Big((-x)^{-2\beta} - B^2\Big)\Big(2B^2 \frac{\hat{\lambda}_R}{\rho_{0R}} + \hat{\nu}_R\Big((-x)^{-2\beta} - B^2\Big)\Big) + \ldots \tag{17}$$

In summary, our numerical solution of eq. (4) gives a very detailed picture of the critical equation of state. The numerical uncertainties are estimated by comparison of results obtained through two independent integration algorithms [8]. They are small, typically less than 0.3% for critical exponents and 1 − 3% for amplitudes. The scaling relations between the critical exponents are fulfilled within a deviation of 2×10^{-4}. The dominant quantitative error stems from the truncation of the exact flow equation and is related to the size of the anomalous dimension $\eta \simeq 4\%$. This is consistent with the fact that the critical exponents and amplitudes calculated here typically deviate by a few percent from the more precise values obtained by other methods [3]. If the equation of state is needed with a higher accuracy one has to extend the truncation beyond the level of the present work.

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Tables

N	β	γ	δ	ν	η	λ_R/m_R	ν_R	$\hat{\lambda}_R/\rho_{0R}$	$\hat{\nu}_R$	
1	0.336	1.258	4.75	0.643	0.044	9.69	108	61.6	107	
3	0.388	1.465	4.78	0.747	0.038	7.45	57.4	0	$\simeq 250$	
	C^+	D	B	ξ^+	E	C^+/C^-	ξ^+/ξ^-	R_χ	$\tilde{R}_\xi$	ξ^+E
1	0.0742	15.88	1.087	0.257	0.652	4.29	1.86	1.61	0.865	0.168
3	0.0743	8.02	1.180	0.263	0.746	-	-	1.11	0.845	0.196

Table 1: Parameters for the equation of state.

Figures

Fig. 1 : Logarithmic plot of f and df/dx for $x > 0$.

Fig. 2 : Logarithmic plot of f and df/dx for $x < 0$.