On a trivial aspect of canonical specific heat scaling

Michael Promberger
Institut für Theoretische Physik, Universität Erlangen-Nürnberg,
Staudtstrasse 7, D–91058 Erlangen, Germany

Abstract. We show that the canonical finite size scaling of the specific heat emerges naturally – and in some sense trivially – from the assumption that the microcanonical specific entropy exhibits no substantial system size dependence.

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1 Introduction

Since the introduction of the Renormalization–Group by Wilson [1], we have learned much about critical phenomena and the striking feature of universality. Unfortunately, the majority of systems with nontrivial behaviour cannot be treated analytically. Nevertheless, there exist approximation schemes concerning finite systems which allow to estimate the properties of the corresponding infinite system by proper extrapolation to the thermodynamic limit. A very powerful method for the investigation of the critical properties of an infinite system along these lines is the so-called finite size scaling theory introduced by Fisher et al. (see [2], [3] and references therein). Although hypothesised before the advent of the Renormalization–Group, finite size scaling may be understood within the framework of the latter.

The main result of finite size scaling theory may be stated like this: In the vicinity of the critical point of a given infinite system, the system size dependence of certain thermal properties of the corresponding finite system is governed by properties (namely: the critical indices) of the infinite system. Or, formulated slightly differently: In spite of the fact, that the free energy density of a finite system is a completely analytic function of its variables, the system size dependence of certain derivatives of the free energy density are dictated by quantities which describe the non–analytic behaviour of the free energy density of the corresponding infinite system.

All thermal properties of a finite system (volume \( V \equiv N := L^d \)) are given by logarithmic derivatives of the canonical partition function

\[
Z_N(T) := \sum_{x \in \Gamma} e^{-\beta H(x)} , \quad T = \frac{1}{\beta} , \quad k_B \equiv 1 ,
\]

where \( H(x) \) represents the energy of a particular microstate \( x \) of the system and the sum runs over all possible microstates which constitute the space \( \Gamma \) of all the states available to the system. With the definition of the microcanonical density of states

\[
\Omega_N(\varepsilon) := \sum_{x \in \Gamma} \delta_{H(x),N\varepsilon}
\]

and the microcanonical specific entropy

\[
\hat{s}_N(\varepsilon) := \frac{1}{N} \ln \Omega_N(\varepsilon) ,
\]

the canonical partition function reads

\[
Z_N(T) := \sum_{\varepsilon} e^{N(\hat{s}_N(\varepsilon) - \beta \varepsilon)} .
\]

\(^1\)Throughout this paper, we will use the language of lattice systems with discrete energies, where the number of degrees of freedom \( N \) is equivalent to the volume \( V \).
Here, the sum runs over all possible energy-values of the finite system. As it is clearly visible, the system size dependence of the partition function is due to two causes. Namely, the size dependence of the microcanonical specific entropy \( \hat{s}_N(\varepsilon) \) and the overall factor \( N \) in the exponential, which we will call the trivial system size dependence.

It is the aim of this paper to demonstrate that finite size scaling emerges naturally and in some sense trivially from the assumption that the critical properties of the infinite system are already contained in the microcanonical specific entropy of the finite system. Unfortunately, up to now we are able to show this only as far as the finite size scaling properties of the specific heat are concerned.

Although we are never introducing a specific system explicitly by giving its Hamiltonian, we restrict our discussion to systems with short range interactions. For this reason, standard finite size scaling is applicable and hyperscaling holds. \(^2\)

Remark: In the thermodynamic limit, the entropy \( \hat{s}_N(\varepsilon) \) is replaced by the Massieu–function \( \hat{s}(\varepsilon, h/T) \) at zero magnetic field \( h \) (=: \( \hat{s}(\varepsilon) \)), which is the Legendre transform of the entropy \( s(\varepsilon, m) \):

\[
\lim_{N \to \infty} \hat{s}_N(\varepsilon) = \hat{s}(\varepsilon, \frac{h}{T} = 0) = \sup_m \left\{ s(\varepsilon, m) + \frac{h}{T} m \right\}_{\frac{h}{T} = 0} \]

Here, \( m \) denotes the magnetization per particle. In this paper, the thus defined Massieu–function will be called ”microcanonical specific entropy”.

In section 2, we give an explicit form for the microcanonical specific entropy of a system which undergoes a continuous phase transition with a power law singularity of the specific heat. In section 3, we show that the system size independence of the microcanonical specific entropy implies canonical finite size scaling. Namely, the scaling of the specific heat maximum (section 3.1) and the scaling of the softening of the specific heat singularity (section 3.2). Since we are not able to proof the reverse direction of this statement, in section 4, we give some hints onto the validity of the conjecture that the system size dependence of the microcanonical specific entropy is such weak not to impact the canonical finite size scaling.

### 2 Microcanonical specific entropy vs. continuous phase transitions

The microcanonical specific entropy of a system which undergoes a continuous phase transition may be written as a sum of a singular part \( \hat{s}_{\text{sing}}(\varepsilon) \) and a correction term \( \hat{s}_{\text{corr}}(\varepsilon) \) which is needed to correctly describe the behaviour of the specific heat at least if the dimensionality of the system is smaller than the upper critical dimension of the corresponding universality–class.
entropy outside the critical region.

\[ \hat{s}(\varepsilon) = \hat{s}_{\text{sing}}(\varepsilon) + \hat{s}_{\text{corr}}(\varepsilon) \]  \hspace{1cm} (6)

If the corresponding specific heat shows a power law singularity, the choice

\[ \hat{s}_{\text{sing}}(\varepsilon) = \hat{s}_c + \beta_c (\varepsilon - \varepsilon_c) - \frac{\beta_c |\varepsilon_c|}{g} |\varepsilon - \varepsilon_c|^g \left( \Theta(\varepsilon_c - \varepsilon) A + \Theta(\varepsilon - \varepsilon_c) A' \right) \]  \hspace{1cm} (7)

(with \( g := \frac{2-\alpha}{1-\alpha} \)) for the singular part of the specific entropy yields the correct behaviour of the singular part of the specific heat. \( \hat{s}_c, \varepsilon_c \) and \( \beta_c \) are the values of the specific entropy, the specific energy and the inverse temperature at the critical point (\( \beta_c := 1/T_c \)), the step-function \( \Theta(x) \) is defined by \( \Theta(x) := 1 \forall x > 0 \) and \( \Theta(x) := 0 \forall x \leq 0 \). Indeed, since the microcanonical specific heat is given by

\[ c(\varepsilon) := -\frac{\beta(\varepsilon)^2}{s''(\varepsilon)} := -\frac{s'(\varepsilon)^2}{s''(\varepsilon)} \]  \hspace{1cm} (8)

differentiating the singular part (7) of the specific entropy twice with respect to the specific energy \( \varepsilon \) yields

\[ c_{\text{sing}}(\varepsilon) = \frac{\beta_c |\varepsilon_c|}{g - 1} \left( \frac{\Theta(\varepsilon_c - \varepsilon)}{A} + \frac{\Theta(\varepsilon - \varepsilon_c)}{A'} \right) |\varepsilon - \varepsilon_c|^{-\frac{\alpha}{1-\alpha}} \]  \hspace{1cm} (9)

in the vicinity of the critical point \( \varepsilon_c \). Alternatively, by going over from \( \frac{\varepsilon - \varepsilon_c}{\varepsilon_c} \) to \( \frac{T-T_c}{T_c} \) via

\[ \left| \frac{\beta(\varepsilon) - \beta_c}{\beta_c} \right| \approx \left| \frac{\varepsilon - \varepsilon_c}{\varepsilon_c} \right|^{-\frac{\alpha}{1-\alpha}} \left( \Theta(\varepsilon_c - \varepsilon) A + \Theta(\varepsilon - \varepsilon_c) A' \right) \]  \hspace{1cm} (10)

the singular part of the microcanonical specific heat as a function of the reduced temperature \( t := (T - T_c)/T_c \) is proportional to \( |t|^{-\alpha} \):

\[ c_{\text{sing}}(t) = (1 - \alpha) \frac{|\varepsilon_c|}{T_c} \left( \frac{\Theta(T_c - T)}{A^{1-\alpha}} + \frac{\Theta(T - T_c)}{A'^{1-\alpha}} \right) |t|^{-\alpha} \]  \hspace{1cm} (11)

The correction term \( \hat{s}_{\text{corr}}(\varepsilon) \) of the specific entropy yields no contribution to the singular behaviour of the specific heat if it obeys the following condition:

\[ \lim_{\varepsilon \to \varepsilon_c} \frac{\hat{s}_{\text{corr}}(\varepsilon)}{|\varepsilon - \varepsilon_c|^g} = 0 \]  \hspace{1cm} (12)

\(^3\) In the case of a logarithmic singularity the last term in \( \hat{s}_{\text{sing}}(\varepsilon) \) should be replaced by a function of the form \( (\varepsilon - \varepsilon_c)^2 / \ln |\varepsilon - \varepsilon_c| \).
3  Microcanonical specific entropy vs. finite size scaling of the canonical specific heat

In the rest of this paper, we will study finite size scaling properties of the canonical specific heat of a hypothetical $N$–particle system with specific entropy

$$\hat{s}_N(\varepsilon) \equiv \hat{s}_{\text{sing}}(\varepsilon) + \hat{s}_{\text{corr},N}(\varepsilon) \quad \forall \ N > N_0$$  \hspace{1cm} (13)

This implies the assumption that, at least for sufficiently large $N$, the singular contribution to $\hat{s}_N(\varepsilon)$ is identical to the singular part of the entropy of the infinite system. The correction term $\hat{s}_{\text{corr},N}(\varepsilon)$ may show some $N$–dependence which should of course be consistent with the condition (12).

Having postulated the form of the entropy in (13) the canonical specific heat $c_N(T)$ of the $N$–particle system follows directly from (4). We shall compare the scaling properties of the thus determined specific heat $c_N(T)$ with the results of conventional finite size scaling theory [5]. At the critical temperature $T_c$ of the infinite system the finite size scaling theory predicts for the value of the specific heat of the finite system

$$c_N(T_c) \propto L^{\frac{d}{2} - \alpha}$$  \hspace{1cm} (14)

In the finite system the singularity is smeared. Scaling theory predicts for the width of the specific heat anomaly:

$$\Delta T(L) \propto \left( \frac{1}{L} \right)^{\frac{1}{\nu}}$$  \hspace{1cm} (15)

Here, $\nu$ is the critical exponent of the correlation length $\xi(t)$ of the infinite system, $L$ is the linear dimension of the finite system and $T_c$ denotes the critical temperature of the infinite system.

We are now going to show, that the finite size scaling relations

$$c_N(T_c) \propto L^{\frac{d}{2} - \alpha}$$  \hspace{1cm} (16)

and

$$\Delta T(L) \propto \left( \frac{1}{L} \right)^{\frac{1}{\nu}}$$  \hspace{1cm} (17)

are direct consequences of the postulate (13). Together with the validity of hyperscaling, (16) implies (14) and (17) implies (15). While (17) is established by numerical integration, (16) can be shown analytically.

3.1  Canonical specific heat scaling at $T_c$

The first step consists in the calculation of the $n$–th moment of the specific energy of the $N$–particle system with respect to the canonical distribution at the critical
temperature of the infinite system.

$$\langle \varepsilon^n \rangle_N(T_c) = \frac{1}{Z_N(T_c)} \sum_{\varepsilon} \varepsilon^n e^{N(\delta_N(\varepsilon) - \beta_c \varepsilon)}$$  \hspace{1cm} (18)

$Z_N(T_c)$ denotes the canonical partition function of the $N$-particle system at $T_c$ (cf. (13)). For sufficiently large $N$, it is justified to replace the sum over all possible energy-values by an integration along the energy-axis. Since the correction term $\delta_{corr, N}(\varepsilon)$ of the specific entropy will yield no contribution to the canonical quantities at $T_c$ (for sufficiently large $N$ again), we are concerned with integrals of the type

$$I_n := \int_{-\infty}^{\infty} d\varepsilon \varepsilon^n \exp \left\{ -N \frac{\beta_c |\varepsilon_c|}{g} \left| \frac{\varepsilon - \varepsilon_c}{\varepsilon_c} \right|^g \left( \Theta(\varepsilon_c - \varepsilon) A + \Theta(\varepsilon - \varepsilon_c) A' \right) \right\}$$  \hspace{1cm} (19)

Defining new amplitudes $B := A\beta_c|\varepsilon_c|^{-g}/g$, $B' := A'\beta_c|\varepsilon_c|^{-g}/g$ and renaming $(\varepsilon - \varepsilon_c) \rightarrow \varepsilon$, we get

$$I_n = \sum_{l=0}^{n} \binom{n}{l} \varepsilon_c^{n-l} \int_{0}^{\infty} d\varepsilon \varepsilon^l \left( e^{-NB'\varepsilon^g} + (-1)^l e^{-NB\varepsilon^g} \right)$$  \hspace{1cm} (20)

Substituting $x := NB'\varepsilon^g$ in the first and $x := NB\varepsilon^g$ in the second term of the integral, we end up with the following expression for $I_n$:

$$I_n = \sum_{l=0}^{n} \binom{n}{l} \frac{\varepsilon_c^{n-l}}{g} \left( B'^{l+1} - (-1)^l B^{-l+1} \right) N^{-\frac{l+1}{g}} \int_{0}^{\infty} dx x^{\frac{l+1}{g}-1} e^{-x}$$  \hspace{1cm} (21)

Since we want to study the finite size scaling properties of the canonical specific heat $c_N(T)$

$$c_N(T_c) := N\beta_c^2 \left( \langle \varepsilon^2 \rangle_N(T_c) - \langle \varepsilon \rangle^2_N(T_c) \right)$$  \hspace{1cm} (22)

at the critical temperature $T_c$ of the infinite system, we have to look at the second central moment of the specific energy with respect to the canonical distribution:

$$\langle \varepsilon^2 \rangle_N(T_c) - \langle \varepsilon \rangle_N^2(T_c) = \frac{I_2}{I_0} - \left( \frac{I_1}{I_0} \right)^2 =$$

$$= N^{-\frac{2}{g}} \left[ \frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} \frac{B'^{-\frac{4}{9}} + B^{-\frac{4}{9}}}{B'^{-\frac{4}{9}} + B^{-\frac{4}{9}}} - \frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} \frac{B'^{-\frac{4}{9}} + B^{-\frac{4}{9}}}{B'^{-\frac{4}{9}} + B^{-\frac{4}{9}}} \right]^2 \propto N^{-\frac{2}{g}}$$  \hspace{1cm} (23)

With $g := (2 - \alpha)/(1 - \alpha)$ and $N = L^d$, $d$ being the dimension of configuration space, eq. (14) follows immediately from (23). In conjunction with the hyperscaling relation

$$d\nu = 2 - \alpha$$  \hspace{1cm} (24)

this implies (14).
3.2 Scaling of the specific heat width $\Delta T$

The specific heat singularity (11) of the infinite system is rounded in the corresponding finite systems. Since in the canonical ensemble there are no phase transitions in finite systems, this effect seems to be quite natural. The standard (finite size scaling) argument for this softening is that the specific heat of the finite system saturates for those temperatures, where the correlation length $\xi(t)$ of the infinite system becomes larger than the linear system size $L$. The correlation length $\xi_N(t)$ of the finite system is bounded from above by a length which is of the order of magnitude of the linear system size $L$. For this reason, there is a temperature region within which the specific heat of the finite system deviates essentially from the specific heat of the infinite system.

Any measure of the width of this region will do. For numerical convenience, the width $\Delta T(L)$ is defined as the temperature range where $c_N(T)$ is larger than 80% of its maximum value. Having defined $\Delta T(L)$, it is an easy matter to compute it by numerical integration via eqs. (4) and (7) for any lattice size $L$. The various parameters appearing in (7) have not been chosen arbitrarily but we have taken the parameter set obtained by a fit to the (simulated) entropy data of a three-dimensional Ising model with linear system size $L = 18$. The parameters are:

$\varepsilon_c = -1.059; \alpha = 0.1155; \beta_c = 0.222684; A = 0.091; A' = 0.150$.

Fig. 1 shows a log–log plot of $\Delta T(L)$ vs. $1/L$ where we have chosen $N = L^3 = 10^8, ..., 10^{10}$ together with a straight–line fit to the data points. The critical exponent $(2 - \alpha)/d$, which is just the inverse slope of the fitted straight line (cf. (17)), emerges to be $(2 - \alpha)/d = 0.6275$ which is consistent with the value of $\nu = 0.6282$ obtained by combining the input–value of $\alpha = 0.1155$ with the hyperscaling relation (24).

4 On the system size dependence of microcanonical specific entropies

In the previous section, we have shown that a system size independent microcanonical specific entropy implies the canonical finite size scaling relations. Unfortunately, we are not able to proof this statement in the reverse direction. Nevertheless, we can report at least two observations which are necessary (not sufficient) for the validity of the statement that the system size dependence of the microcanonical specific entropy has no considerable impact on canonical finite size scaling (if the systems are not chosen to be too small).

1) If the microcanonical specific entropy shows no system size dependence and if the critical properties of the infinite system are already contained in the entropy of $\hat{s}_c$, the value of $\hat{s}_c$ is not listed, because an additive constant in the specific entropy is quite irrelevant with respect to the physics described by that entropy. Likewise the value of $\varepsilon_c$ is irrelevant for the smearing.

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the corresponding finite systems, then it should be possible to extract information about the critical exponent $\alpha$ by performing some fits of a function of the form (4) to the entropy data of finite systems obtained by, e.g., Monte Carlo simulation. And indeed, it has already been shown [4], that an entropy of the form (6) with the singular part given in (7) fits the data of a $10 \times 10 \times 10$–Ising system very well and it will be shown elsewhere, that the same entropy with the same exponent $g$ but slightly modified parameters $\varepsilon_c$, $\beta_c$ is well suited to fit the data of larger 3D–Ising systems (the values of the critical exponent $\alpha$ emerging from this fits is well consistent with the respective value of $\alpha$ in the thermodynamic limit, i.e. $\alpha_{\text{fit}} \in [0.08; 0.12]$).

2) If the microcanonical specific entropy shows no substantial system size dependence, then it should make no difference if the value of the specific heat of a finite system at the critical temperature of the infinit system is calculated by use of the entropy of the finite system or by use of the entropy of the infinit system. Fortunately, this can be checked in the case of the twodimensional Ising model, where the entropy of the infinit system can be calculated from Onsagers solution [3]. At zero external field, the internal energy per particle as a function of the inverse temperature reads as:

$$
\epsilon(\beta) = -\coth(2\beta) \left[ 1 + \frac{2}{\pi} \left( 2 \tanh^2(2\beta) - 1 \right) K_1(q) \right]
$$

(25)

where

$$
q := \frac{2 \sinh(2\beta)}{\cosh^2(2\beta)} \quad \text{and} \quad K_1(q) := \int_0^{\pi/2} d\varphi \left( 1 - q^2 \sin^2 \varphi \right)^{1/2}, \quad J \equiv k_B \equiv 1.
$$

(26)

Here, $J$ denotes the Ising coupling constant. Since the inverse temperature $\beta$ is defined to be the derivative of the entropy $\hat{s}(\varepsilon)$ with respect to the energy $\varepsilon$, the entropy can be calculated according to

$$
\hat{s}(\varepsilon) = \text{const.} + \int_{\varepsilon_0}^{\varepsilon} d\tilde{\varepsilon} \beta(\tilde{\varepsilon})
$$

(27)

with arbitrary $\varepsilon_0$. $\beta(\varepsilon)$ is obtained by inverting eq. (25). In the case of a logarithmic specific heat singularity, the canonical finite size scaling theory predicts

$$
c_N(T_c) \propto \ln(1/L)
$$

(28)

Having obtained the entropy of the infinit 2D Ising system, it is an easy thing to calculate the critical point specific heat using eq. (22). The result is shown in figure 2.
5 Conclusion

We have shown that the finite size scaling relations (16) and (17) are trivial consequences of the postulate (13): for sufficiently large \( N \), the entropy of the finite system was assumed to be identical to the entropy of the infinite system at least in the vicinity of the critical point. In this context, ”trivial” means that the softening of the specific heat singularity is caused solely by the trivial factor \( N \) in the exponential of the canonical partition function (4). In the framework of this scenario it is therefore not astonishing that some properties of the finite system are governed by the critical indices of the infinite system: they are already contained in the entropy of the finite system but they are covered up by the averaging (”smearing”) procedure of the canonical partition function (for a detailed discussion of this ”smearing–effect” see [8]). For this reason it seems to be plausible that, as far as finite systems are concerned, we are in some sense blinded by the canonical formalism which obscures the information already available in the microcanonical specific entropy.

Indeed, the hypothetical system which we have discussed may seem to be a rather strange construction but it is not as arbitrary as it seems to be since we have already shown that an entropy of the type (7) is well suited to fit the data of a \( 10^3 \)-3d–Ising system. Note that this is by no means the only example of a system with a microcanonical specific entropy \( s_N(\varepsilon) \) which shows no substantial \( N \)–dependence. We will report about other examples elsewhere.

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References

[1] K. G. Wilson and J. Kogut; Phys. Rep. 12C, 75 (1974)
[2] M. E. Fisher and M. N. Barber; Phys. Rev. Lett 28, 1516 (1972)
[3] M. N. Barber in; ”Phase Transitions and Critical Phenomena” Vol. 8 edited by Domb/Lebowitz, Academic Press (1983), pp 146
[4] M. Promberger and A. Hüller; Z. Phys. B 97, 341 (1995)
[5] K. Binder; in "Finite Size Scaling and Numerical Simulation of Statistical Systems" edited by V. Privman, World Scientific (1990), pp 173

[6] L. Onsager, Phys. Rev. 65, 117 (1944)

[7] A.E. Ferdinand and M.E. Fisher; Phys. Rev. 185, 832 (1969)

[8] A. Hüller; Z. Phys. B 93, 401 (1994)
Fig. 1 log–log plot of $\Delta T(L)$ vs. $1/L$ for system sizes $N = L^3 = 10^8, ..., 10^{10}$. A straight–line fit to the data points yields $(2 - \alpha)/d = 0.6275$ which is consistent with the predicted value of $\nu = 0.6282$. 

Captions
