Critical properties of the spherical model in the microcanonical formalism

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Abstract. Due to the equivalence of the statistical ensembles, thermostatic properties of physical systems with short-range interactions can be calculated in different ensembles leading to the same physics. In particular, the ensemble equivalence holds for systems that undergo a continuous phase transition in the infinite volume limit with the result that the properties of the transition can also be investigated in the microcanonical approach. Considering as an example the spherical model, the ensemble equivalence is explicitly demonstrated by calculating the critical properties in the microcanonical ensemble and comparing them to the well known canonical results.

Keywords: solvable lattice models, classical phase transitions (theory), critical exponents and amplitudes (theory)
1. Introduction

The properties of physical systems exhibiting a continuous (or discontinuous) phase transition are usually investigated in the canonical approach. However, for systems with short-range interactions the various physical ensembles such as the canonical ensemble and the microcanonical one are equivalent in the infinite volume limit with the result that the properties of continuous phase transitions can be investigated in the microcanonical ensemble as well\(^1\). The microcanonical description is based on the entropy, as the thermodynamic potential and the physical properties of the system are deduced from its geometry. Microcanonical response functions, for example, are related to the curvature of the entropy surface.

The description of phase transitions in the microcanonical formalism has gained growing interest in recent years (see [2]–[6] and references therein). Apart from works about discontinuous phase transitions in microcanonical systems [7]–[9], [5, 10, 11, 6, 12] second-order phase transitions have been studied recently [4], [13]–[19]. Ways to extract critical exponents from microcanonical quantities calculated for finite systems have also been suggested and applied successfully for various model systems [14, 15, 20, 21]. All these works basically concentrate on signatures of phase transitions in finite systems although some works investigated the general scaling behaviour of the entropy of the infinite system near a continuous transition [14, 22].

\(^1\) It should be noted that the ensembles are inequivalent at a first-order transition point even if the interactions are short ranged. This subtle difference is exploited for the study of phase separation in microcanonical systems (e.g. [1]).

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The main purpose of this paper is to demonstrate the equivalence of the microcanonical and the canonical ensemble in the infinite system for a concrete example of a model system with short-range interactions that undergoes a second-order phase transition and can be tackled analytically. To this end the properties of the spherical model at the phase transition point are investigated within the microcanonical ensemble. By doing this it is also shown as an example that the investigation of continuous phase transitions is not restricted to the canonical ensemble and can be carried out beneficially in the microcanonical ensemble, too. There are only a few model systems with short-range interactions and a phase transition in the thermodynamic limit which, within the framework of the canonical ensemble, have been solved exactly. The zero-field Ising model in two dimensions and the spherical model in all dimensions belong to the class of models where the free energy density of the infinite system is known analytically. As far as I am aware, a microcanonical investigation of a model system with short-range forces exhibiting a non-trivial continuous phase transition in the thermodynamic limit has not been reported in the literature yet. Here, an investigation of the interrelation of the canonical and microcanonical critical exponents of the spherical model is carried out. As the natural variables are different for the microcanonical and the canonical ensemble, the critical exponents are in general not identical. The equivalence of the ensembles, however, leads to a relation between them. Note that this relation was discussed in [26] for statistical ensembles whose thermodynamic potentials are connected to each other by Legendre transforms. The entropy, as the thermodynamic potential of the microcanonical ensemble, however, is related, for instance, to the free energy by a Legendre transform and a subsequent partial inversion. The results for the microcanonical spherical model presented in this paper corroborate general considerations that have been based on scaling relations for the microcanonical entropy function [14,22].

The rest of the paper is organized as follows. In section 2 a brief introduction to the microcanonical analysis of physical properties of ferromagnetic systems is given. This section also sets up the notation and language used later on. The specific entropy of the ferromagnetic spherical model is calculated in section 3 in the macroscopic limit using the method of steepest descent. The critical properties of the spherical model are then analysed microcanonically in section 4 with special focus on the values of the microcanonical critical exponents. Section 5 contains some comments on the mean spherical model. The findings are summarized and compared to the canonical results in the final section 6.

2. Thermostatics in the microcanonical formalism

The basic quantity in the investigation of the statistical properties of a finite magnetic system with \( N \) particles is the density of states

\[
\Omega_N(E, M) = \int d\Gamma_N \delta(E - \mathcal{H}(\sigma))\delta(M - \mathcal{M}(\sigma)).
\]  

(1)

The Hamiltonian \( \mathcal{H} \) provides the energy for any microstate \( \sigma = (\sigma_1, \ldots, \sigma_N) \) from the phase space \( \Gamma_N \) of all possible configurations of the \( N \)-particle system. The magnetization

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\(^2\) See for instance [23, 24, 12, 25] for recent investigations of the question of the equivalence of the microcanonical and the canonical ensemble for systems with long-range forces.
The microcanonical entropy density of a finite magnetic system with $N$ particles is obtained from the density of states by taking the logarithm

$$s_N(e, m) = \frac{1}{N} \ln \Omega_N(eN, mN) \quad (2)$$

where the energy density is defined by $e = E/N$; analogously, the magnetization density is given by $m = M/N$. Note that units with $k_B = 1$ are used in this work. The thermodynamic properties of the system in the thermodynamic limit are calculated from the entropy

$$s(e, m) = \lim_{N \to \infty} s_N(e, m). \quad (3)$$

The thermostatics of an infinite system can be investigated by studying the free energy as the thermodynamic potential with the temperature being one of the natural variables or alternatively by considering the entropy where the energy shows up as a natural variable [27]. In the following it is briefly summarized how the physical properties of statistical systems can be deduced from the entropy function $s(e, m)$. The inverse temperature $\beta(e, m)$ and the magnetic field $h(e, m)$ are basically given by the first derivatives of the entropy function:

$$\beta(e, m) = \frac{\partial}{\partial e} s(e, m) \quad (4)$$

and

$$h(e, m) = -(\beta(e, m))^{-1} \frac{\partial}{\partial m} s(e, m). \quad (5)$$

Note that the inverse temperature $\beta$ and the magnetic field $h$ show up as conjugate variables to the natural variables $e$ and $m$ in the microcanonical ensemble.

The zero-field macrostate $(e, m_{sp}(e))$ is defined to be the state with zero magnetic field $h(e, m_{sp}(e)) = 0$ for given energy $e$. The associated magnetization $m_{sp}(e)$ is called spontaneous magnetization. The corresponding inverse temperature is defined to be $\beta_0(e) = \beta(e, m_{sp}(e))$. The response functions of the system are related to second-order derivatives of the entropy function [14, 17, 21]. The specific heat for the zero-field macrostate, for instance, is explicitly given by

$$c_0(e) = -\frac{(\beta_0(e))^2}{(\partial/\partial e)\beta_0(e)}. \quad (6)$$

In the vicinity of a critical point, which shows up at a critical energy $e_c$, the physical quantities display power-law behaviour. Denoting the deviation of the energy $e$ from the critical value $e_c$ by $\varepsilon := e - e_c$, a general physical quantity $a$ has the form $a(e) \sim |\varepsilon|^{-\zeta}$ for small $\varepsilon$. The singularity of $a$ is characterized by the critical exponent $\zeta$, which characterizes the singularity of
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The critical exponent of the specific heat in the canonical formalism is denoted by $\alpha_t$ and has to be in the interval $[0, 1]$ for relation (7) to be valid [4]. If the specific heat in the canonical formalism has a jump singularity, a logarithmic singularity or a cusp singularity at the transition point the microcanonical and canonical critical exponents are identical.

As this paper considers the spherical model, which has a cusp singularity in the specific heat, the case of a cusp singularity is briefly sketched. In the vicinity of the transition point the canonical specific heat with a cusp at the transition temperature $T_c$ has the general form

$$c^{(c)} \sim A + B_{\pm} |t|^{-\alpha_t}$$

with $t := T - T_c$ and a negative canonical exponent $\alpha_t$. Integrating expression (8) gives

$$\varepsilon \sim At - \frac{B_{\pm}}{1 + |\alpha_t|} |t|^{1 + |\alpha_t|}.$$  

The dominating term in the limit $t \to 0$ is thus the linear term and one has $\varepsilon \sim t$ near the transition point. Therefore, physical quantities have the same qualitative dependence when expressed as functions of the reduced temperature $t$ or the reduced energy $\varepsilon$. The critical exponents are consequently identical for the canonical and microcanonical descriptions.

The exponent $\delta_\varepsilon$ describes the relation between the critical magnetic field and the magnetization at the transition energy (or temperature). The microcanonical exponent is therefore always identical to the canonical exponent $\delta_t$.

3. Specific entropy of the spherical model

In this section the density of states of the spherical model [28] is calculated for finite systems. The spherical model exhibits a continuous phase transition and can be solved analytically for an arbitrary magnetic field in any dimension $d$. Therefore, its critical properties have been studied intensively within the canonical ensemble in the past (see e.g. [29]–[31]). From the density of states one gets the specific entropy of the infinite lattice by taking the thermodynamic limit (3). The density of states will be evaluated for a hypercubic system in $d$ dimensions with a linear extension $L$ so that the system contains $N = L^d$ spins. The spin variables $\sigma_i \in \mathbb{R}$, $i = 1, \ldots, N$, can take on any real value, but they have to satisfy the constraint

$$\sum_{i=1}^{N} \sigma_i^2 = N.$$  

The phase space of the spherical model is therefore the sphere of radius $\sqrt{N}$ in $\mathbb{R}^N$. The integration measure in the definition (1) of the density of states is just given by the Lebesgue measure $d\Gamma_N = d^N \sigma$. The Hamiltonian of the spherical model is given by

$$\mathcal{H}(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$
with a positive exchange constant $J$; the magnetization is

$$M(\sigma) = \sum_i \sigma_i.$$  

(12)

The angular brackets $\langle i, j \rangle$ indicate a summation over all neighbouring lattice sites $i$ and $j$. The Hamiltonian (11) together with the subsidiary condition (10) defines the ferromagnetic spherical model with nearest neighbour interactions only.

The density of states of the spherical model is generally given by

$$\Omega_N(E, M) = \int_{\mathbb{R}^N} d^N \sigma \delta(E - H(\sigma)) \delta(M - M(\sigma)) \delta\left(N - \sum_i \sigma_i^2\right).$$

(13)

In view of the three delta functions, the integral remains unchanged if one inserts the factors $\exp(aE - aH(\sigma))$, $\exp(bM - bM(\sigma))$ and $\exp(cN - c\sum_i \sigma_i^2)$ with real $a$, $b$ and $c$. Using the Fourier representation

$$\delta(x) = \int \frac{dk}{2\pi} \exp(ikx)$$

(14)

of the delta function one can rewrite the expression for the density of states as

$$\Omega_N(E, M) = \int \frac{dp}{2\pi} \int \frac{dq}{2\pi} \int \frac{dr}{2\pi} \int d^N \sigma \exp(A_{p,q,r}(\sigma)),$$

(15)

where the argument $A$ of the exponential is given by

$$A_{p,q,r}(\sigma) = (a + ip)E + (b + iq)M + (c + ir)N + Q_{p,q,r}(\sigma)$$

(16)

with the quadratic form

$$Q_{p,q,r}(\sigma) = (a + ip)\sum_{\langle i,j \rangle} \sigma_i \sigma_j - (c + ir)\sum_i \sigma_i^2 - (b + iq)\sum_i \sigma_i^2$$

$$= -\sigma^T W\sigma + v^T \sigma.$$

(17)

The last equality defines the matrix $W$, which describes the interaction of the spins; the vector $v$ is the vector in $\mathbb{R}^N$ which has $N$ identical entries $-(b + iq)$. The transpose of a vector $v \in \mathbb{R}^N$ is denoted by $v^T$. Introducing new spin variables $\mu \in \mathbb{R}^N$ via

$$\mu = \sigma - \frac{1}{2}W^{-1}v,$$

(18)

the form $Q$ is given by

$$Q_{p,q,r}(\mu) = -\mu^T W \mu + \frac{1}{2}v^T W^{-1} v$$

(19)

in terms of the new variables $\mu$ (provided the inverse $W^{-1}$ exists). The spin variables $\mu$ appear now quadratically so that one is left with a multiple Gaussian integral yielding

$$\Omega_N(E, M) = \int \frac{dp}{2\pi} \int \frac{dq}{2\pi} \int \frac{dr}{2\pi} \exp(\Phi_{p,q,r}(E, M))$$

(20)

with the argument

$$\Phi_{p,q,r}(E, M) = (c + ir)N + (a + ip)E + (b + iq)M + \frac{1}{2}v^T W^{-1}v - \frac{1}{2} \ln \det W.$$

(21)

Here the identity $(\det W)^{-1/2} = \exp(-1/2 \ln \det W)$ has been used.

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The interaction matrix $W$, that has been defined in expression (17), is a generalized cyclic matrix, which can be diagonalized by a Fourier transformation in any dimension $d$ (e.g. [30, 31]). For the case of nearest neighbour interactions only, one gets the eigenvalues

$$\lambda(\varphi_1, \ldots, \varphi_d) = (c + ir) - (a + ip)J \sum_{j=1}^{d} \cos \varphi_j$$

(22)

with $\varphi_j = (l-1)2\pi/L$, $l = 1, \ldots, L-1$ and $j = 1, \ldots, d$. The logarithm of the determinant of $W$ is now given by

$$\ln \det W^{\sim 1} N \int_{[0,2\pi]^d} \frac{d^d\varphi}{(2\pi)^d} \ln \left( (c + ir) - (a + ip)J \sum_{j=1}^{d} \cos \varphi_j \right)$$

(23)

where the summation has been replaced by an integral in the macroscopic limit of asymptotically large $N$ (i.e. large $L$). As $v$ is an eigenvector of $W$ with the eigenvalue $(c + ir) - (a + ip)dJ$ it is also an eigenvector of the inverse $W^{-1}$ with the eigenvalue $((c + ir) - (a + ip)dJ)^{-1}$. Therefore, one has

$$\frac{1}{4} v^T W^{-1} v = \frac{N}{4((c + ir) - (a + ip)dJ)}(b + iq)^2.$$  

(24)

Introducing the new integration variables $z = a + ip$, $w = b + iq$ and $u = c + ir$ the density of states is now given by

$$\Omega_N(Ne, Nm) = \lim_{N \to \infty} \int_{a-i\infty}^{a+i\infty} \frac{dz}{2\pi} \int_{b-i\infty}^{b+i\infty} \frac{dw}{2\pi} \int_{c-i\infty}^{c+i\infty} \frac{du}{2\pi} \exp(N\phi_{z,w,u}(e,m))$$

(25)

with the argument

$$\phi_{z,w,u}(e,m) = ze + wm + u - \frac{1}{2} \int \frac{d^d\varphi}{(2\pi)^d} \ln \left( u - zJ \sum_{j} \cos \varphi_j \right) + \frac{w^2}{4(u - zdJ)}.$$  

(26)

This expression for the density of states for asymptotically large $N$ can be used now to calculate the specific entropy of the infinite system by using the method of steepest descent [32]. The argument of the logarithm in (26) must have a strictly positive real part for any possible value of the $\varphi_j$. Therefore, the real part of $u$ has to be positive. If $\text{Re}z \in ]-\text{Re}u/(dJ), \text{Re}u/(dJ)[$ the function $\phi$ is analytic in $z$, $w$ and $u$ in this domain. Consider the function $\phi$ first for real values of $z$, $w$ and $u$. For $w \to \pm \infty$ one has $\phi \to \infty$ and for $z \to \pm u_0/(dJ)$ one also has $\phi \to \infty$. The function $\phi$ has therefore a minimum for a real $w_0$, $z_0$ and $u_0$ with $z_0 \in ]-u_0/(dJ), u_0/(dJ)[$. Due to the analyticity of $\phi$ the integration path can now be deformed to have $a = z_0$, $b = w_0$ and $c = u_0$ so that one obtains

$$s(e, m) = \lim_{N \to \infty} \frac{1}{N} \ln \Omega_N(eN, mN) = \phi_{z_0,w_0,u_0}(e,m)$$

(27)

for the specific entropy in the thermodynamic limit, by the method of steepest descent. The values $z_0$, $w_0$ and $u_0$ as functions of the energy $e$ and the magnetization $m$ are
determined by the saddle point equations
\[
\frac{\partial \phi}{\partial z} = e + \frac{1}{2} \int \frac{d^d\varphi}{(2\pi)^d} \frac{J \sum_j \cos \varphi_j}{u - zJ \sum_j \cos \varphi_j} + \frac{dJ}{4(u - zJ)^2} w^2 = 0, \tag{28}
\]
\[
\frac{\partial \phi}{\partial w} = m + \frac{1}{2(u - zJ)} w = 0 \tag{29}
\]
and
\[
\frac{\partial \phi}{\partial u} = 1 - \frac{1}{2} \int \frac{d^d\varphi}{(2\pi)^d} \frac{1}{u - zJ \sum_j \cos \varphi_j} - \frac{1}{4(u - zJ)^2} w^2 = 0. \tag{30}
\]

4. Critical properties of the spherical model

In this section the physical properties of the spherical model are deduced directly from the specific entropy (27). The main focus is on the possible appearance of a continuous phase transition signalled, for example, by diverging response functions. In particular, the character of the singular physical quantities at the phase transition point which shows up in dimensions larger than two will be scrutinized. As the entropy of the spherical model is an even function in \(m\) the discussion will consider only non-negative magnetizations.

4.1. Discussion of the saddle point equations

The microcanonical inverse temperature of the spherical model is given by
\[
\beta(e, m) = \frac{\partial s(e, m)}{\partial e} = \frac{\partial \phi}{\partial e} + \frac{\partial \phi}{\partial z} \frac{\partial z}{\partial e} + \frac{\partial \phi}{\partial w} \frac{\partial w}{\partial e} + \frac{\partial \phi}{\partial u} \frac{\partial u}{\partial e} = \frac{\partial \phi}{\partial e} = z_0(e, m) \tag{31}
\]
where the saddle point equations (28)–(30) have been used for the last but one equality. Similarly, the microcanonical magnetic field is determined by
\[
h(e, m)\beta(e, m) = -\frac{\partial}{\partial m}s(e, m) = -w_0(e, m). \tag{32}
\]
Defining the new function \(\zeta(e, m) := u_0(e, m)/z_0(e, m)\), the saddle point equation (29) can be re-expressed as
\[
h(e, m) = 2m(\zeta(e, m) - dJ). \tag{33}
\]
Note that the variable \(\zeta(e, m)\) has to be larger than the critical value \(\zeta_c := dJ\) due to the restrictions for the argument of the logarithm in (26). The relation (33) can be used now to rewrite the other two saddle point equations (28) and (30):
\[
\beta(e, m) \left[ e + dJm^2 \right] = -\frac{1}{2} \int \frac{d^d\varphi}{(2\pi)^d} \frac{J \sum_j \cos \varphi_j}{\zeta(e, m) - J \sum_j \cos \varphi_j} \tag{34}
\]
and
\[
\beta(e, m) \left[ 1 - m^2 \right] = \frac{1}{2} \int \frac{d^d\varphi}{(2\pi)^d} \frac{1}{\zeta(e, m) - J \sum_j \cos \varphi_j} =: R(\zeta(e, m)). \tag{35}
\]
In the following the system for a fixed energy $e$ is considered for the limit of vanishing (positive) magnetic field $h \to 0^+$, i.e. for the zero-field macrostate $(e, m_{sp}(e))$. The corresponding zero-field inverse temperature is defined to be $\beta_0(e) = \beta(e, m_{sp}(e))$; analogously $\zeta_0(e) = \zeta(e, m_{sp}(e))$. In the limit $m \to m_{sp}(e)$ (corresponding to $h(e, m) \to 0^+$ for fixed energy $e$) one gets the equation

$$m_{sp}(e)(\zeta_0(e) - dJ) = 0 \tag{36}$$

which has to be obeyed by the spontaneous magnetization. This equation has the trivial solution $m_{sp}(e) = 0$. A non-zero spontaneous magnetization is only possible if the bracket in (36) vanishes, i.e. if $\zeta_0 = dJ$. Therefore, a non-zero spontaneous magnetization below some critical energy $e_c$ is only possible if $\zeta_0(e) = dJ$ for $e < e_c$.

The possible emergence of a non-zero spontaneous magnetization is further discussed in section 4.2. Before this consideration can be carried out it has to be investigated whether it is possible at all to have a critical energy $e_c$ larger than the ground state energy $e_g = -dJ$ so that $\zeta_0(e) = dJ$ holds below $e_c$. To this end consider first the second relation (35) and assume that there exists a critical energy $e_c$ above which the spontaneous magnetization $m_{sp}(e)$ vanishes. Then one must have $\zeta_0(e) > dJ$ for $e > e_c$ and the associated inverse temperature $\beta_0(e) = \beta(e, m_{sp}(e) = 0)$ of the zero-field macrostates ($e > e_c, 0$) is given by $\beta_0(e) = R(\zeta(e, 0))$ (see relation (35) for the definition of $R$). In view of equation (36) a non-zero spontaneous magnetization can appear for energies below the critical value only if $\zeta_0(e) = dJ$ for all $e < e_c$. At the critical energy $e_c$ one therefore has $\zeta(e_c) = \zeta_c$ and the associated critical inverse temperature $\beta_c$ is thus given by $\beta_c = R(\zeta_c)$. In the limit $\varphi_j \to 0$, $j = 1, \ldots, d$, the sum $\sum_j \cos \varphi_j$ tends to $d$ and thus the vanishing denominator in (35) might cause a diverging integral for the limit $\zeta_0 \to \zeta_c$. This would have the consequence that the critical inverse temperature $\beta_c$ is infinite so that the model has no phase transition. To investigate this situation more explicitly consider the contributions to the integral which arise from small $\varphi_j$. In the regime $\varphi_j \to 0$ the denominator can be approximated by $\frac{1}{2}(\varphi_1^2 + \cdots + \varphi_d^2)$. Introducing polar coordinates for the $d$-dimensional $\varphi$-space and excluding a small sphere of radius $\delta$ from the integration over $\varphi_j$, $j = 1, \ldots, d$, one gets the factor

$$-\lim_{\delta \to 0} \int_{\delta} d\varphi \varphi^{d-3} \tag{37}$$

to which the dominant small $\varphi_j$ contributions to the integral $R$ are proportional. The modulus of the vector $(\varphi_1, \ldots, \varphi_d)$ is here denoted by $\varphi$. For one and two dimensions the limit (37) diverges and one has $\beta_c = \infty$ and the spherical model does not undergo a phase transition in these dimensions. From equation (34) it is evident that the associated critical energy $e_c = -dJ$ is the ground state energy of the spherical model. For dimensions larger than two the limit (37) exists and hence the (critical) inverse temperature $\beta_c$ is finite and the model will have a phase transition at some energy $e_c > -dJ$ (see subsequent subsections).

### 4.2. Spontaneous magnetization

This subsection discusses how a microcanonical spontaneous magnetization can emerge in the spherical model for dimensions larger than two. Consider first the case of $d \leq 2$ for the
limit \( m \to m_{\text{sp}}(e) \). The function \( R \) for the zero-field macrostate is shown schematically in figure 1. Below the critical value \( \zeta_c = dJ \) the integral \( R \) is not defined. Above \( dJ \) the spontaneous magnetization that is associated with \( \zeta_0 \) has to vanish in order to satisfy equation (36). On approaching \( dJ \) from above, \( R(\zeta_0) \) diverges and therefore one always has \( \beta_0 = R(\zeta_0) \) (compare equation (35)) and no spontaneous magnetization can emerge. The situation for \( d > 2 \) is also displayed in figure 1. In contrast to the case for \( d \leq 2 \) the integral \( R \) approaches a finite value \( R(\zeta_c) \) in the limit \( \zeta_0 \to dJ \). If the inverse temperature \( \beta_0 \) is chosen to be above \( R(\zeta_c) = \beta_c \) (or equivalently \( e < e_c \)) the saddle point equation (35) can only be satisfied if a non-zero spontaneous magnetization \( m_{\text{sp}}(e) \) shows up\(^3\). This is possible if \( \zeta_0(e) = dJ \) for \( e < e_c \) so that the subsidiary condition (36) holds. Saddle point equation (35) now reduces to

\[
m_{\text{sp}}(e) = \sqrt{\frac{\beta_0(e) - \beta_c}{\beta_0(e)}}.
\] (38)

The critical energy on the other hand is given by \( e_c = P(\zeta_c)/\beta_c \) (see relation (34) for the definition of \( P \)) and below \( e_c \) the saddle point equation (34) for the zero-field macrostate is just \( \beta_0(e + dJm_{\text{sp}}^2) = e_c \beta_c \). This equation can now be used to eliminate \( \beta_0 \) from (38) and one has

\[
m_{\text{sp}}(e) = \sqrt{\frac{e_c - e}{e_c + dJ}}.
\] (39)

The spontaneous magnetization is therefore characterized by the critical exponent \( \beta_c = 1/2 \) for all dimensions \( d > 2 \). Note, however, that relation (39) is valid for all energies below the critical one. At the ground state energy \( e_g = -dJ \) the spontaneous magnetization is one as expected.

At this stage it should be remarked that the entropy \( s(e,m) \) does exist for the spontaneous magnetization \( m_{\text{sp}}(e) \) although the argument of the logarithm in (26) then vanishes. The investigation of physical properties corresponding to derivatives of the entropy function gives sensible results for the limit \( m \to m_{\text{sp}}(e) \). Note that similarly the free energy of the spherical model in the canonical formalism is also defined for zero magnetic field (i.e. for the spontaneous magnetization) for temperatures below the critical one (e.g. [31,33]).

4.3. Specific heat for dimensions \( d > 2 \)

The two saddle point equations (34) and (35) for the zero-field macrostate contain the spontaneous magnetization which can be zero or non-zero depending on whether the energy is above or below the critical value \( e_c \). Equation (35) can be used to eliminate the magnetization from relation (34) yielding

\[
e = \frac{1}{2} \int \frac{d^d \phi}{(2\pi)^d} \frac{dJ}{\zeta_0(e)} - J \sum_j \cos \varphi_j \frac{1}{\beta_0(e)} - dJ.
\] (40)

\(^3\) In the microcanonical ensemble the energy \( e \) is the natural variable and the associated inverse temperature \( \beta_0(e) \) for the zero-field macrostate is determined by the integral equations (34) and (35). As the specific heat in the infinite system has a well defined sign, however, the inverse temperature \( \beta_0 \) can be chosen first and from the saddle point equations the associated energy \( e \) can be calculated in principle, finally yielding the desired function \( \beta_0(e) \).
Below $e_c$ one has $\zeta_0 = dJ$ so that

$$
e = \frac{1}{2} \frac{1}{\beta_0(e)} - dJ = \frac{1}{2} T_0(e) - dJ$$

where $T_0(e) = 1/\beta_0$ is the actual temperature associated with the zero-field macrostate $(e, m_{sp}(e))$. Thus, the microcanonical specific heat is a constant, namely $c_0 = 1/2$, for all energies below $e_c$ and all dimensions $d > 2$.

For arbitrary energies the microcanonical specific heat (6) of the spherical model is given by

$$c_0(e) = \frac{1}{2} \int \frac{d^d\varphi}{(2\pi)^d} \frac{dJ - J \sum_j \cos \varphi_j}{\zeta_0(e) - J \sum_j \cos \varphi_j} + \frac{1}{2} \frac{dJ}{\zeta_0(e)} - J \sum_j \cos \varphi_j)^2 \frac{d\zeta_0}{d\beta_0}$$

for the zero-field macrostate in view of equation (40). For $e < e_c$ the expression (42) reduces to the result already discussed above as $d\zeta_0/d\beta_0 = 0$. In the limit $\zeta_0 \to \zeta_c^+$ from above, the two integrals that appear in (42) both approach finite values which can be seen by a similar analysis carried out for the investigation of the behaviour of the integral $R$ in this limit. The behaviour of the specific heat for the regime $e \to e_c^+$ corresponding to $\zeta_0 \to \zeta_c$ is thus determined by the behaviour of the derivative $d\zeta_0/d\beta_0$.

As a first step for the analysis of the limit $e \to e_c^+$, i.e. $\varepsilon \to 0+$, define for the zero-field macrostate the new variables $\tau := \beta_\varepsilon - \beta_0$ and $\xi := \zeta_0 - \zeta_c$. Then $\tau = R(\zeta_c) - R(\zeta_0)$ for energies above the critical value and one has the asymptotic relations

$$\tau = R(\zeta_c) - R(\zeta_0) \sim \begin{cases} 
\xi^{(d-2)/2} & \text{if } 2 < d < 4, \\
-\xi \ln \xi & \text{if } d = 4, \\
\xi & \text{if } d > 4
\end{cases}$$

for the limit $\xi \to 0+$ [29]–[31]. The deviation of the energy from the critical energy is given by

$$\varepsilon = e - e_c = \frac{P(\zeta_0(e))}{\beta_0(e)} - \frac{P(\zeta_c)}{\beta_\varepsilon} \sim \frac{\tau P(\zeta_c)}{\beta_\varepsilon^2} + \frac{1}{\beta_\varepsilon} (P(\zeta_0(e)) - P(\zeta_c)).$$

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The two differences $P(\zeta_0) - P(\zeta_c)$ and $R(\zeta_0) - R(\zeta_c)$, however, have the same asymptotic behaviour for $\xi \to 0^+$ as the two integrals $P$ and $R$ differ only in the numerator which does not alter the asymptotic behaviour for $\xi \to 0^+$. Thus, one has $\varepsilon \sim \tau$ near the critical point. Note that at this stage it is already obvious that the critical exponents of the spherical model are the same for the canonical and the microcanonical ensemble.

Using these results and the relation

$$
\frac{d\zeta_0}{d\beta_0} = \frac{d\xi}{d\beta_0} = \frac{d\xi}{d\tau}
$$

one obtains the following asymptotic relations for the microcanonical specific heat near the transition point:

$$
c_0(\varepsilon) \sim \begin{cases} 
1/2 - A_d \xi^{-(d-4)/2} & \text{if } 2 < d < 4, \\
1/2 - B_d |\ln \varepsilon| & \text{if } d = 4, \\
1/2 - B_d & \text{if } d > 4
\end{cases}
$$

(46)

where $A_d$ and $B_d$ are some constants. In the analysis of the regime $e \to e_c$ the first integral in (42) has been replaced by $1/2$. Note that the correction term originating from this integral in (42) does not contribute to the leading asymptotic behaviour of the microcanonical specific heat. For dimensions $2 < d \leq 4$ the form (46) of the microcanonical specific heat is characterized by the negative critical exponent $\alpha_{\varepsilon} = (d - 4)/(d - 2)$ corresponding to a (right-sided) cusp singularity. For dimensions $d > 4$ the microcanonical specific heat has a discontinuity at the transition point.

4.4. Susceptibility

The susceptibility is generally defined by

$$
\chi = \frac{dm}{dh} = \left( \frac{dh}{dm} \right)^{-1}
$$

(47)

Focusing on energies $e > e_c$ and using the general relation (32) between the magnetic field and the magnetization one gets the microcanonical susceptibility

$$
\chi_0(e) = \frac{1}{2(\zeta_0(e) - dJ)} = \frac{1}{2\xi}
$$

(48)

for the zero-field macrostate. Expressing this in terms of the energy deviation $\varepsilon$ one gets thus the asymptotic relations

$$
\chi_0(e) \sim \begin{cases} 
\varepsilon^{-2/(d-2)} & \text{if } 2 < d < 4, \\
(\varepsilon/|\ln \varepsilon|)^{-1} & \text{if } d = 4, \\
\varepsilon^{-1} & \text{if } d > 4
\end{cases}
$$

(49)

for the microcanonical susceptibility in the regime $\varepsilon \to 0^+$. The microcanonical exponent of the susceptibility in $2 < d < 4$ space dimensions is therefore $\gamma_{\varepsilon} = 2/(d - 2)$ and in dimensions $d \geq 4$ one has the microcanonical exponent $\gamma_{\varepsilon} = 1$. 

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4.5. Critical field

At the critical energy $e_c$ the saddle point equation (35) reduces to

$$\beta(e_c, m) = R(\zeta_c + h(e_c, m)/(2m))$$  \hspace{1cm} (50)

where relation (32) has been used to eliminate $\zeta$ from equation (35). Carrying out the asymptotic analysis of $R$ for the limit $m \to m_{sp}(e_c) = 0$ one gets the values

$$\delta_e = \begin{cases} 
\frac{d + 2}{d - 2} & \text{if } 2 < d < 4, \\
3 & \text{if } d \geq 4
\end{cases}$$  \hspace{1cm} (51)

for the critical field exponent $\delta_e$.\(^4\)

5. Mean spherical model

The calculations presented in the above sections showed that the thermodynamic properties of the spherical model are equivalent in the canonical and microcanonical ensembles as far as the spontaneous magnetization, the susceptibility, the specific heat and the critical field are concerned. This is apparent at first sight from the corresponding expressions for these quantities. In the microcanonical ensemble the energy and the magnetization are fixed to some values. These constraints are represented by the first two delta functions in the expression (13) for the density of states. These two constraints can be relaxed so that they are only satisfied on average. This corresponds to the canonical treatment where the Lagrange parameters which are then introduced to satisfy the constraints on the energy and magnetization turn out to be related to the temperature and the magnetic field, respectively. In a similar way the spherical constraint (10) can be relaxed so that it is only satisfied on average (the model is then often called the mean spherical model). Lewis and Wannier used this relaxation to calculate the properties of the canonical spherical model [34]. However, it turned out that the properties of the mean spherical model are only partially equivalent to the properties of the spherical model with the rigid constraint (10), as quantities which are related to the fluctuations in the spherical constraint are different for the spherical and mean spherical models [35, 36, 33, 37]. These differences have their origin in the fact that the Lagrange parameter that controls the constraint in the mean spherical model does not have a corresponding variable in the spherical model. Note that this is different for the Lagrange parameters temperature and magnetic field in the canonical ensemble which have corresponding variables, namely the energy and the magnetization.

A similar treatment can be carried out in the microcanonical ensemble. The spherical constraint can be relaxed and controlled by a Lagrange parameter so that it is satisfied on average. Only two delta functions, namely those which fix the energy and the magnetization, are left in the expression for the density of states and therefore only relations (28) and (29) show up as saddle point equations in the thermodynamic limit. However, the requirement that the spherical constraint is satisfied on average leads to a subsidiary condition which fixes the Lagrange parameter introduced. This additional

\(^4\) Note that the analysis of the exponent $\delta_e$ is similar to the canonical analysis of $\delta_t$ (see e.g. [31]) and is therefore not displayed here.
subsidiary condition is identical to relation (30) and therefore the investigated properties of the microcanonical spherical model and the microcanonical mean spherical model are equivalent. Nevertheless, the relaxation of the spherical constraint now allows for fluctuations in this constraint and having the canonical results in mind it might be expected that differences will occur when comparing quantities that are related to those fluctuations. This interesting question goes beyond the scope of the present work and is left to future studies.

6. Summary

The various statistical ensembles are equivalent for systems with short-range interactions undergoing a continuous phase transition in the infinite volume limit. Therefore, physical quantities can be calculated in different ensembles leading to the same thermodynamic properties. The properties of a model system undergoing a continuous phase transition in the thermodynamic limit can hence be directly deduced from the microcanonical entropy. As an example the spherical model was investigated microcanonically in this work to demonstrate these general properties and to provide an analytic treatment of a model system within the microcanonical formalism. The calculation of the microcanonical entropy as presented in section 3 somewhat resembles the determination of the free energy in the canonical treatment (see e.g. [30]). This already hints at the equivalence of the microcanonical and the canonical treatment of the spherical model. However, in the microcanonical calculation further saddle point equations emerge due to the restrictions on the energy and the magnetization represented by the delta functions in (13). To establish ensemble equivalence for the spherical model explicitly, these additional saddle point equations have to be analysed as is done in section 4.

The natural variables of the canonical and microcanonical formalism are different so one gets in general different critical exponents for physical quantities. However, the canonical and microcanonical critical exponents are related to each other to ensure ensemble equivalence. In the case of a cusp singularity in the specific heat at the transition point the microcanonical and the canonical critical exponents are identical whereas the exponents are different for systems with an algebraically diverging specific heat (compare relation (7)). The spherical model is a system with such a cusp singularity in the specific heat. The microcanonical critical exponents are therefore expected to be identical to the canonical critical exponents. This was indeed verified explicitly in this work.

The microcanonical treatment of the spherical model on an infinite hypercubic lattice carried out in this work also demonstrates how properties of physical systems near a continuous phase transition point can be deduced directly from the density of states (or equivalently the microcanonical entropy) without going to the canonical ensemble.

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