Entropy and specific heat of a critical quantum system with long-range interaction

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Abstract. The entropy and the specific heat of a quantum spherical model with a long-range interaction (decreasing at large distances \( r \) as \( r^{-d-\sigma} \) where \( d \) is the space dimensionality and \( 0 < \sigma \leq 2 \)) are studied in the quantum critical region at the upper quantum critical dimension \( d = 3\sigma/2 \). The problem of obtaining the temperature-dependent corrections to the ground state free energy involves the solution of a transcendental equation, the exact solution of which is expressed in terms of the Lambert W-function. The free energy, the entropy and the specific heat in the quantum critical region are derived in terms of the Lambert W-function.

For systems in real physical dimensions (chains, thin layers, i.e. films and three-dimensional systems) the exact results for the entropy and the specific heat obtained in terms of the Lambert W-function and the leading asymptotic ones are compared on the basis of the calculated relative errors. It can be concluded that for a class of quantum models at the upper critical dimension the Lambert W-function is a very effective tool for an exact computation of low-temperature critical properties, especially in the finite-temperature quantum critical region.

1. Introduction

The aim of this study is to obtain the entropy and the specific heat of a critical quantum system in the finite-temperature quantum critical region at the upper quantum critical dimension.

The model considered here is a quantum version of the spherical model or more precisely the "spherical quantum rotors" model (SQRM) [1]. Its equivalence with the quantum nonlinear \( O(n) \) sigma model (QNL\( \sigma \)M) [2–5], widely used in the exploration of the critical behavior of quantum magnets, in the limit \( n \rightarrow \infty \) is shown in [1]. The mathematical analogy between the SQRM and a modification of the \( \varphi^4 \) lattice model used extensively in studying the structural phase transitions (see e.g. [6] and references therein) is discussed in [7]. In [1] the critical exponents of the SQRM for both the zero-temperature quantum critical point and the finite-temperature classical one as functions of the dimensionality have been obtained. Due to its exact solvability for each dimensionality the SQRM is very useful for analytical research of the scaling properties of quantum critical phenomena and of finite-size effects [7–9].

In the framework of the model of structural phase transitions, mentioned above, it has been shown that the Lambert W-function [10] is a very effective tool for an exact computation of non-universal critical properties in the neighborhoods of both the classical and the quantum critical points at the corresponding upper critical dimensions [11, 12]. In [13] the specific heat of the classical mean-spherical model has been exactly calculated in terms of the Lambert W-function.

In this paper, using the properties of the Lambert W-function we study the entropy and the specific heat of the SQRM in the quantum critical region at the upper quantum critical dimension.
2. The model

The Hamiltonian of the model is [1]

\[ H = \frac{1}{2} g \sum_i p_i^2 - \frac{1}{2} \sum_{i,l'} J_{i,l} S_i S_{l'} + \frac{1}{2} \mu \sum_i S_i^2 - h \sum_i S_i, \]

where \( S_i \) are spin operators at site \( i \). The operators \( P_i \) play the role of "conjugated" momenta (i.e. \( [S_i, S_{i'}] = 0, [P_i, P_{i'}] = 0, \) and \( [P_i, S_{i'}] = i \delta_{ii'} \), with \( h = 1 \)). The coupling constant \( g \) measures the strength of the quantum fluctuations (below, it will be called quantum parameter), \( J_{l,l'} = J(r) \) is the interaction matrix between spins at sites \( l \) and \( l' \), \( h \) is an ordering magnetic field, and the spherical field \( \mu \) is introduced so as to ensure the constraint

\[ \sum_i \langle S_i^2 \rangle = N. \]

Here \( N \) is the total number of quantum spins located at sites "\( l \)" of a \( d \)-dimensional hypercubical lattice and \( \langle \ldots \rangle \) denotes the standard thermodynamic average taken with the Hamiltonian (1). The commutation relations for the operators \( S_i \) and \( P_i \) together with the kinetic term in the Hamiltonian (1) do not describe quantum Heisenberg-Dirac spins but quantum rotors as is pointed out in [1].

The considered here long-range interaction potential \( J(r) \sim r^{-d-\sigma} \), where \( \sigma > 0 \) and \( r \to \infty \), enters the exact expression for the free energy of the model only through its Fourier transform [14]. The long-wavelength (small \( k \equiv |k| \)) leading asymptotic of its Fourier transform is \( U(k) \cong J |k|^\sigma, 0 < \sigma < 2 \), where the energy scale has been fixed so that \( U(0) = 0 \). The case \( \sigma \geq 2 \) corresponds to short-range interaction, i.e. the universality class then does not depend on \( \sigma \). Values satisfying \( 0 < \sigma < 2 \) correspond to long-range interactions and the critical behavior depends on \( \sigma \).

The normalized free energy density \( \tilde{f} = f / J \) of the model (1) in the thermodynamic limit \( N \to \infty \) at \( h = 0 \) has the form [9]

\[ \tilde{f}(t, \lambda |d, \sigma) = \sup_{\phi} \{ t k_d \int_0^{x_d} x^{d-1} \ln \left[ 2 \sinh \left( \frac{\lambda}{2 t} \sqrt{\phi + x^\sigma} \right) \right] dx - \frac{\phi}{2} \} - d, \]

where the supremum in the equation (3) is attained at the solutions of the mean-spherical constraint, equation (2), that is obtained by differentiating the above expression with respect to \( \phi \)

\[ 1 = \frac{\lambda}{2} k_d \int_0^{x_d} \frac{x^{d-1}}{\sqrt{\phi + x^\sigma}} \coth \left( \frac{\lambda}{2 t} \sqrt{\phi + x^\sigma} \right) dx. \]

In equations (3) and (4) we have introduced the notations: \( \lambda = \sqrt{g/J} \) is the normalized quantum parameter, \( t = T/J \) - the normalized temperature, \( \phi = \mu/J \) - the scaled spherical field, \( k_d^{-1} = \frac{1}{2} (4 \pi)^{\frac{d}{2}} \Gamma (d/2) (\Gamma \) is the Euler gamma function and \( x_d = 2 \pi (d / S_d)^{1/d} \) is the radius of the sphericalized Brillouin zone, \( S_d = 2 \pi^{d/2} / \Gamma (d/2) \). From the condition that in the quantum critical point \( (\lambda = \lambda_c, t = 0) \) the solution of (4) is \( \phi = 0 \), one obtains the critical value \( \lambda_c, \lambda_c = (2 - \sigma / d) x_d^{\sigma / 2} \).

Equations (3) and (4) provide the basis for studying the bulk critical behavior of the model.

In this paper we shall consider the entropy and the specific heat capacity in the quantum critical region \( (\lambda = \lambda_c) \) at the upper quantum critical dimension \( d = 3 \sigma / 2 \). In the neighborhood of the quantum critical point, by using the exact solution of the spherical field equation (4) in terms of the Lambert W-function, we establish exact analytical expressions for the free energy density, the entropy and the specific heat capacity. When the upper critical dimension coincides with real physical dimensions (chains, thin layers, i.e. films and three-dimensional systems), the obtained exact results for the specific heat are compared with the leading asymptotic ones on the basis of the calculated relative errors.
3. Temperature-dependent corrections to the free energy density at the quantum critical point

In the low-temperature limit \( t \ll 1 \) replacing \( \frac{1}{t} x D^{\sigma/2} \) by infinity at \( d = 3\sigma/2 \) the above expression for the free energy density (3) takes the form

\[
\tilde{f}(t, \lambda | \sigma) = \sup_{\phi} \left\{ \frac{1}{x D} \frac{\lambda}{\lambda_c} \left[ 2 \frac{2}{3} x D^{\sigma/2} (\phi + x D^{\sigma}) \right]^{1/2} F \left( -\frac{1}{2}, 1; \frac{5}{2}, \frac{x D^{\sigma}}{\lambda_c} + \phi \right) + 4 \left( \frac{t}{\lambda} \right)^{4} \Phi(\phi) \right\} - \frac{\phi}{2} \right\} - \frac{3}{2} \sigma,
\]

(5)

where \( F(a, b; c; x) \) is the hypergeometric function and

\[
\Phi(\phi) = \int_{0}^{\infty} x^2 \ln \left[ 1 - \exp \left( -\frac{\lambda^2}{t^2} \phi + x^2 \right) \right] \, dx.
\]

(6)

Sufficiently close to the quantum critical point \( \phi \ll 1 \) the integral (6) can be evaluated as \( \Phi(\phi) = \Phi(0) + \Phi'(0) \phi \) and retaining the leading terms, including \( \phi^2 \ln \phi \)-term, after some algebra, we can write (5) in the form

\[
\tilde{f}(t, \lambda | \sigma) = \tilde{f}_c + \frac{1}{2} \left( \frac{\lambda}{\lambda_c} - 1 \right) \phi + A \phi^2 \ln \phi + B t^4 + C t^2 \phi,
\]

(7)

where \( \tilde{f}_c = x D^{\sigma/2} - 3\sigma/2 \) is the free energy density at the quantum critical point,

\[
A = \frac{1}{\left[ 6(4\pi)^{3/4} \sigma^{2} \Gamma \left( \frac{3}{2} \sigma \right) \right]^{2/3}},
\]

(8)

\[
B = - \frac{18 \zeta(4)}{2(4\pi)^{3/4} \sigma^{2} \Gamma \left( \frac{3}{2} \sigma \right)}.
\]

(9)

and

\[
C = \frac{3 \zeta(2)}{\left[ \sqrt{6}(4\pi)^{3/4} \sigma^{2} \Gamma \left( \frac{3}{2} \sigma \right) \right]^{4/3}},
\]

(10)

\( \zeta(x) \) is the Riemann zeta function. In (7) \( \phi \) is the solution of the corresponding spherical field equation, that reads

\[
\frac{1}{2} \left( \frac{\lambda}{\lambda_c} - 1 \right) + 2A \phi \ln \phi + A \phi + C t^2 = 0.
\]

(11)

At \( \lambda = \lambda_c \), i.e. in the quantum critical region, (11) has the form

\[
\phi \ln \phi + \frac{1}{2} \phi = - \frac{C}{2A} t^2.
\]

(12)

By the substitution \( \ln \phi + 1/2 = W(x) \), the equation (12) takes the form of the defining equation for the Lambert W-function [10],

\[
W(x) \exp (W(x)) = x.
\]

(13)

When \( x \) is a real variable, then for \(-1/e \leq x < 0\) there are two branches with real values of \( W(x) \): the branch \( W_0(x) \) satisfying \(-1 \leq W_0(x) \) and the branch \( W_{-1}(x) \leq -1 \), as \( \lim_{x \to -0} W_{-1}(x) = -\infty \). Thus, in terms of the Lambert W-function, the exact solution of (12) is

\[
\phi = \exp \left[ W_{-1} (-\epsilon) - 1/2 \right],
\]

(14)
Figure 1. The coefficient $B$ as a function of $\sigma$, i.e. of the dimensionality of the system.

where $\epsilon_t = (C/2A)\sqrt{\epsilon t^2}$. The choice of the solution $W_1(x)$ corresponds to the fact that at the quantum critical point ($\lambda = \lambda_c, t = 0$) the scaled spherical field $\phi$ vanishes.

By using the convergent series for the branch $W_1(-x)$ at small $x > 0$ [10] and retaining the leading two terms, we get the asymptotic expression for $\phi$,

$$\phi \approx -\frac{C}{A}t^2 \ln t.$$ \hspace{1cm} (15)

Let us note that for a wide class of models the logarithmic behavior of the susceptibility $\chi = \phi^{-1}$ is well known in the theory of phase transitions (see, e.g. [6]).

At $\lambda = \lambda_c$ near to the quantum critical point, by substituting (14) into (7), we get the following exact expression for the temperature-dependent corrections to the free energy density at the quantum critical point

$$\tilde{f}(t, \lambda_c | \sigma) - \tilde{f}_c = B t^4 \left[ 1 + \frac{5}{4} W_{-1}(\frac{1}{\epsilon_t}) + \frac{5}{8} W_{-1}^2(\frac{1}{\epsilon_t}) \right].$$ \hspace{1cm} (16)

The asymptotic expression for the temperature-dependent corrections to the free energy density at the quantum critical point can be obtained by substituting (15) into (7). It is easy to see that the coefficient $B$, given by (9), characterizes the leading $t$-corrections to the ground state free energy of the system at its quantum critical point. The coefficient $B$ as a function of $\sigma$ is graphically presented on figure 1.

4. Derivatives of the free energy with respect to the temperature - entropy and specific heat

By using (7) and taking into account the spherical field equation (12), for the entropy, $S$, and the specific heat, $c$, per spin in the quantum critical region ($\lambda = \lambda_c$) near to the quantum critical point we have

$$S = -\frac{\partial \tilde{f}}{\partial t} = -4B t^3 - 2C t \phi.$$ \hspace{1cm} (17)

and

$$c = t \frac{\partial S}{\partial t} = -12B t^3 - 2C t \phi - 2C t^2 \frac{d \phi}{dt}.$$ \hspace{1cm} (18)
Substituting in (17) and (18) the exact solution for $\phi$, given by (14), we obtain the following exact expressions

$$S = -4Bt^3 \left[ 1 + \frac{5}{4} \frac{1}{W_{-1}(-\epsilon_t)} \right]$$  \hspace{1cm} (19)

and

$$c = -12Bt^3 \left[ 1 + \frac{5}{12} \frac{1}{W_{-1}(-\epsilon_t)} + \frac{5}{6} \frac{1}{(1 + W_{-1}(-\epsilon_t))} \right].$$  \hspace{1cm} (20)

From (19) and (20), by using the series for the Lambert W-function [10] we get the leading asymptotic behavior of the entropy and the specific heat as follows

$$S_{\text{appr.}} = -4Bt^3 \left[ 1 + O \left( \frac{5}{8 \ln t} \right) \right]$$  \hspace{1cm} (21)

and

$$c_{\text{appr.}} = -12Bt^3 \left[ 1 + O \left( \frac{5}{8 \ln t} \right) \right].$$  \hspace{1cm} (22)

For systems in real physical dimensions (chains ($\sigma = 2/3$), films ($\sigma = 4/3$) and three-dimensional systems ($\sigma = 2$)) the percent relative errors $|1 - S_{\text{appr.}}/S|$ and $|1 - c_{\text{appr.}}/c|$ as functions of the normalized temperature $t$ and the dimensionality of the system $d$ are graphically presented on figure 2 and figure 3, respectively.

5. Conclusions

In the quantum critical region at the upper quantum critical dimension $d = 3\sigma/2$ exact expressions for the free energy density (16), the entropy (19) and the specific heat (20) of the model (1) are obtained in the Lambert W-function terms. The coefficient $B$, characterizing the leading temperature-dependent corrections to the free energy density at the quantum critical point, is an increasing function of the long-range exponent $\sigma$, i.e. of the dimensionality $d$ of the system (see figure 1).
Figure 3. The percent relative error $|1 - \frac{c_{\text{appr.}}}{c}|$.

Sufficienly close to the quantum critical point the asymptotic results for the entropy, (21), and the specific heat capacity, (22), are applicable. As one can see the critical amplitudes of the entropy and the specific heat capacity are decreasing functions of $\sigma$, i.e. of the dimensionality $d$ of the system. It is not surprising that the critical exponent $\alpha$, characterizing the leading critical behavior of the specific heat, at the upper critical dimension is not depends on $\sigma$ and for the specific heat the Debye law holds, $c \sim t^3$.

From figure 2 and figure 3 it is easy to see that the obtained exact results for the entropy and the specific heat are especially applicable to low-dimensional systems in the finite-temperature quantum critical region.

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