On the Critical Specific Heat of a Quantum System with Long-range Interaction

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Abstract. The specific heat capacity, c, of one infinite d-dimensional quantum system is studied close to the quantum critical point in the framework of the finite-size scaling (FSS) theory for different space dimensionalities $d_l < d < d_u$, where d_l and d_u are the lower and the upper quantum critical dimensions, respectively. A relationship between the critical amplitude of the specific heat and the "temporal" Casimir amplitude, characterizing the leading temperature-dependent corrections to the ground state free energy, is established. In the example of an exactly solvable d-dimensional model with long-range interaction ($0 < \sigma \le 2$ is a parameter controlling the decrease of the long-range interaction), we have obtained the critical amplitude of the specific heat in a simple, analytical, closed form for the special case $d = \sigma$.

Keywords: finite-size scaling, quantum critical region, specific heat capacity, long-range interaction.

1. INTRODUCTION

The specific heat as a measure of the response of the system to a variation of the temperature, on the one hand in the finite-temperature quantum critical region can be experimentally measured, and on the other hand is one of the most intricate thermodynamic quantities to deal with numerical simulations at zero temperature and efficient finite-size scaling (Fytas et al., 2017).

In the context of the finite-size scaling (FSS) theory (Privman & Fisher, 1984) extended to quantum systems (Chamati & Tonchev, 2000) the infinite d-dimensional system at low temperatures close to its zero-temperature critical point g_c (g_c is the critical value of some non-thermal parameter g controlling the phase transition at $T = 0$) is considered as an effective $(d+z)$-dimensional system with d infinite spatial and z finite (temporal) dimensions, where z is the dynamical critical exponent.

The study of the low-temperature specific heat in the framework of the FSS theory enables us to establish a relation with the Casimir effect associated with the emergence of long-range forces caused by the confinement of critical fluctuations of the order parameter (Fisher & Gennes, 1978; Krech, 1994).

The Casimir force in statistical-mechanical systems is characterized by the excess free energy density due to the finite-size contributions to the free energy density of the system. The amplitude of the Casimir interaction, characterizing the leading finite-size corrections to the bulk free energy density at the bulk critical temperature, T_c, is universal, depending on the bulk universality class and the universality classes of the boundary conditions (Krech, 1994).

In an analogy with the "usual" excess free energy density and Casimir amplitude, for a bulk system at low temperatures a "temporal" excess free energy density and "temporal"

Casimir amplitude have been defined in (Chamati et al., 2000).

Here we consider a d-dimensional quantum spherical model with long-range interactions (decreasing at long distances r as $r^{-d-\sigma}$, where $0<\sigma\leq 2$). This model does not describe quantum Heisenberg-Dirac spins, but rather quantum rotors, as it is pointed out in (Vojta, 1996) and it is known as the spherical quantum rotors model (QSRM). The equivalence of the QSRM and the quantum nonlinear $O(n)$ sigma model in its $n\to\infty$ limit is shown in (Vojta, 1996). The spherical approximation (or large n-limit) is a source of tractable models of quantum critical phenomena (Chamati et al., 1997; Chamati et al. 1998; Vojta, 1996; Tu & Weichman, 1994; Nieuwenhuizen, 1995; Nieuwenhuizen & Ritort, 1998).

Due to its exact solvability for each dimensionality the SQRM is very useful for a rigorous study of finite-size effects (Chamati et al., 1997; Chamati et al., 1998; Chamati et al., 2000).

2. A FINITE-SIZE SCALING FORM OF THE SPECIFIC HEAT OF A CRITICAL QUANTUM SYSTEM

Let us consider a d-dimensional infinite quantum system at low temperatures near to its quantum critical point $\left(T=0, g=g_c\right)$ in the absence of an ordering external field for space dimensions $d_l<d<d_u$, where d_l and d_u are the lower and the upper quantum critical dimensions, respectively.

According to the general hypothesis of FSS theory (Privman & Fisher, 1984) extended to quantum systems by (Chamati & Tonchev, 2000), defining the finite size $L_\tau \sim \left(\beta\hbar\right)^{1/z}$, where $\beta = 1/\left(k_B T\right)$, k_B is the Boltzmann constant and $\hbar$ is the reduced Planck constant (in the remainder we will set $\hbar = k_B = 1$), we consider the infinite d-dimensional system as a system with geometry of the form $\infty^d \times L_\tau^z$. If one introduces the scaling variable $x_\tau = L_\tau^{1/\nu}\delta g$, where $\delta g \sim \left(g-g_c\right)/g_c$ is a measure of the deviation from g_c and the critical exponent ν measures the divergence of the correlation length at $T=0$, the singular part of the free energy density, $f_{\text{sing.}}\left(T,\delta g \mid d\right)$, can be written in the scaling form (Chamati & Tonchev, 2000)

$$f_{\text{sing.}}\left(T,\delta g \mid d\right) = T L_\tau^{-d} X\left(x_\tau \mid d\right), \tag{1}$$

while the scaling form of each other physical quantity $\mathcal{A}\left(T, g \mid d\right)$ is

$$\mathcal{A}\left(T,\delta g \mid d\right) = L_\tau^{p}\mathcal{A}_s\left(x_\tau \mid d\right). \tag{2}$$

Here $X\left(x_\tau \mid d\right)$ and $\mathcal{A}_s\left(x_\tau \mid d\right)$ are universal scaling functions, and the parameter p is, the divided by ν, critical exponent measuring the divergence of the thermodynamic function $\mathcal{A}$ at $T=0$ (for the correlation length $p=1$, for the susceptibility $p=\gamma/\nu$, etc.).

For a system close to the critical temperature $T_c \neq 0$, if one introduces $\delta t = \left(T-T_c\right)/T_c$, the specific heat

$$c \approx \frac{\partial^2\left(\beta f_{\text{sing}}\right)}{\partial\left(\delta t\right)^2} \tag{3}$$

behaves like $c \sim \left|\delta t\right|^{-\alpha}$ and the critical exponent α satisfies the hyperscaling relation $2-\alpha = d\nu$.

It can be shown that the susceptibility $\chi_{\delta g}$ associated with the quantum parameter g,

$$\chi_{\delta g}\left(T,\delta g \mid d\right) = \frac{\partial^2\left(\beta f_{\text{sing}}\right)}{\partial\left(\delta g\right)^2}, \tag{4}$$

contains a singular contribution $\chi_{\delta g}\left(T\to +0,\delta g \mid d\right) \sim \left|\delta g\right|^{-\alpha_{\delta g}}$ upon taking

δg through zero, where $\alpha_{\delta g}$ is the specific heat exponent of the equivalent classical problem in $(d+z)$ dimensions (Zaanen et al., 2015). Then for the quantity $\chi_{\delta g}$ it is possible to obtain from Eq. (1) and Eq. (4), in full accordance with Eq. (2), the finite-size scaling form

$$\chi_{\delta g}\left(T,\delta g\,|\,d\right)=L_{\tau}^{\alpha_{\delta g}/\nu}\Xi\left(x_{\tau}\,|\,d\right), \quad (5)$$

where the critical exponent $\alpha_{\delta g}$ satisfies the hyperscaling relation $2-\alpha_{\delta g}=d\nu$ and $\Xi\left(x_{\tau}\,|\,d\right)=d^{2}X\left(x_{\tau}\,|\,d\right)/dx_{\tau}^{2}$ is a universal scaling function which at $x_{\tau}=0$ is $\Xi\left(0\,|\,d\right)=0$.

In obtaining the scaling form of the specific heat it is more convenient to use the relationship

$$c=-\beta^{2}\frac{\partial^{2}\left(\beta f_{\text{sing}}\right)}{\partial\beta^{2}}, \quad (6)$$

which can be written in the form

$$c=-\frac{1}{z^{2}}L_{\tau}^{z+1}\frac{\partial}{\partial L_{\tau}}\left[L_{\tau}^{1-z}\frac{\partial\left(\beta f_{\text{sing}}\right)}{\partial L_{\tau}}\right]. \quad (7)$$

From Eq. (1) and Eq. (7) we obtain the finite-size scaling form of the specific heat

$$c\left(T,\delta g\,|\,d\right)=C_{s}\left(x_{\tau}\,|\,d\right)L_{\tau}^{-d}, \quad (8)$$

where

$$C_{s}\left(x_{\tau}\,|\,d\right)=-\frac{1}{\left(\nu z\right)^{2}}x_{\tau}^{2}\frac{d^{2}X\left(x_{\tau}\,|\,d\right)}{dx_{\tau}^{2}}-\frac{1}{\nu z}\left(\frac{1}{\nu z}-2\frac{d}{z}-1\right)x_{\tau}\frac{dX\left(x_{\tau}\,|\,d\right)}{dx_{\tau}}-\frac{d}{z}\left(\frac{d}{z}+1\right)X\left(x_{\tau}\,|\,d\right) \quad (9)$$

is a universal scaling function.

From Eq. (8) we directly infer that at $g=g_{c}$ $\left(x_{\tau}=0\right)$, i.e. in the quantum critical region, the specific heat is $c\left(T,0\,|\,d\right)\propto T^{d/z}$. For $z=1$ this boils down to the familiar Debye behavior, $c\propto T^{d}$.

When the argument of the scaling functions get replaced by zero $\left(x_{\tau}=0\right)$, we will obtain universal critical amplitudes, characterizing the whole class of universality. The critical amplitude of the free energy density may be interpreted as “temporal” Casimir amplitude, $\Delta_{\text{Cas}}^{t}\left(d\right)$,

$$\Delta_{\text{Cas}}^{t}\left(d\right)=X\left(0\,|\,d\right), \quad (10)$$

which characterizes the leading L_{τ}-corrections to the free energy density at the zero-temperature critical value of the quantum parameter in the absence of an ordering external field (Chamati et al. 2000). From Eq. (9) at $x_{\tau}=0$ we obtain a relationship between the critical amplitude of the specific heat and the “temporal” Casimir amplitude,

$$C_{s}\left(0\,|\,d\right)=-\frac{d}{z}\left(\frac{d}{z}+1\right)\Delta_{\text{Cas}}^{t}\left(d\right). \quad (11)$$

Now we move to study the critical amplitude of the specific heat of one exactly solvable model.

3. THE MODEL

The Hamiltonian of the model in the absence of an ordering external field is (Vojta, 1996)

$$H=\frac{1}{2}g\sum_{l}P_{l}^{2}-\frac{1}{2}\sum_{l,l'}J_{l,l'}S_{l}S_{l'}+\frac{1}{2}\mu\sum_{l}S_{l}^{2}, \quad (12)$$

where S_{l} are spin operators at site l. The operators P_{l} play the role of “conjugated” momenta (i.e. $\left[S_{l},S_{l'}\right]=0$, $\left[P_{l},P_{l'}\right]=0$ and

$[P_l, S_{l'}] = i\delta_{ll'}$). The coupling constant g measures the strength of the quantum fluctuations (below it will be called quantum parameter) and the spherical field μ is introduced so as to ensure the constraint

$$\sum_l \langle S_l^2 \rangle = N . \qquad (13)$$

Here N is the total number of quantum spins located at sites "l" of a d-dimensional hyper-cubical lattice and $\langle ... \rangle$ denotes the standard thermodynamic average taken with the Hamiltonian, Eq. (12).

The considered here long-range interaction enters the exact expression for the free energy of the model only through its Fourier transform (Joyce, 1972). The Fourier transform of the interaction matrix is $U(q) \simeq J|\mathbf{q}|^\sigma \quad (0 < \sigma \le 2)$, where the vector $\mathbf{q}$ has the components $\left\{\frac{2\pi n_1}{L_1}, ..., \frac{2\pi n_d}{L_d}\right\}$, $n_j \in \left\{-\frac{L_j - 1}{2}, ..., \frac{L_j - 1}{2}\right\}$ for L_j odd integers and the energy scale has been fixed so that $U(0) = 0$.

The free energy density of the model, Eq. (12), in the thermodynamic limit $N \to \infty$ has the form (Vojta, 1996)

$$\frac{f}{J} = k_d t \int_0^{x_D} x^{d-1} \ln\left[2\sinh\left(\frac{\lambda}{2t}\sqrt{\phi + x^\sigma}\right)\right] dx - \frac{\phi}{2} - d , \qquad (14)$$

where ϕ are the solutions of the spherical field equation,

$$1 = \frac{\lambda}{2} k_d \int_0^{x_D} \frac{x^{d-1}}{\sqrt{\phi + x^\sigma}} \coth\left(\frac{\lambda}{2t}\sqrt{\phi + x^\sigma}\right) dx . \quad (15)$$

In Eq. (14) and Eq. (15) 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, $x_D = 2\pi(d/S_d)^{1/d}$ is the radius of the sphericalized Brillouin zone, $S_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface of the d-dimensional unit sphere and $k_d^{-1} = (4\pi)^{d/2}\Gamma(d/2)/2$ (Γ is the Euler gamma function).

In the thermodynamic limit it has been shown (Vojta, 1996) that for $d > \sigma$ the long-range order exists at finite temperatures up to a given critical temperature $t_c(\lambda)$.

Here we shall consider the low-temperature region near to the quantum critical point for $\frac{1}{2}\sigma < d < \frac{3}{2}\sigma$, where $\frac{1}{2}\sigma$ and $\frac{3}{2}\sigma$ are the lower and the upper critical dimensions, respectively.

4. A FINITE-SIZE SCALING FORM OF THE FREE ENERGY

From Eq. (14) in the low-temperature limit $(\lambda/t >> 1)$ near to the quantum critical point $(\phi << 1)$ for space dimensions $\frac{1}{2}\sigma < d < \frac{3}{2}\sigma$, for the singular (the ϕ dependent) part of the free energy we obtain

$$\frac{f_{\text{sing}}}{J} = -\frac{\lambda}{2}\left(\frac{1}{\lambda} - \frac{1}{\lambda_c}\right)\phi - \frac{\lambda}{4}\frac{k_d}{\sigma\sqrt{\pi}}\Gamma\left(\frac{d}{\sigma}\right)\Gamma\left(-\frac{d}{\sigma} - \frac{1}{2}\right)\phi^{\frac{d}{\sigma}+\frac{1}{2}} - \frac{\lambda k_d}{\sigma\sqrt{\pi}}\Gamma\left(\frac{d}{\sigma}\right)\phi^{\frac{d}{\sigma}+\frac{1}{2}}\sum_{m=1}^{\infty}\frac{K_{\frac{d}{\sigma}+\frac{1}{2}}\left(m\frac{\lambda}{t}\sqrt{\phi}\right)}{\left(m\frac{\lambda}{2t}\sqrt{\phi}\right)^{\frac{d}{\sigma}+\frac{1}{2}}} , \qquad (16)$$

where ϕ is the solution of the corresponding spherical field equation,

$$\frac{1}{\lambda} - \frac{1}{\lambda_c} = -\frac{k_d}{2\sigma\sqrt{\pi}}\Gamma\left(\frac{d}{\sigma}\right)\left|\Gamma\left(\frac{1}{2} - \frac{d}{\sigma}\right)\right|\phi^{\frac{d}{\sigma}-\frac{1}{2}}$$

$$+\frac{2k_d\Gamma\left(\frac{d}{\sigma}\right)}{\sigma\sqrt{\pi}}\phi^{\frac{d}{\sigma}-\frac{1}{2}}\sum_{m=1}^{\infty}\frac{K_{\frac{d}{\sigma}-\frac{1}{2}}\left(m\frac{\lambda}{t}\sqrt{\phi}\right)}{\left(m\frac{\lambda}{2t}\sqrt{\phi}\right)^{\frac{d}{\sigma}-\frac{1}{2}}}. \qquad (17)$$

In Eq. (16) and Eq. (17) $\lambda_c=(2-\sigma/d)x_D^{\sigma/2}$ is the critical value of the quantum parameter λ at zero-temperature critical point, obtained from Eq.15 after taking the limit $t\to+0$ at $\phi=0$, and $K_\nu(x)$ is the MacDonald function (second modified Bessel function). Let us note that Eq. (16) is a particular case of Eq. (18) in (Chamati et al., 2000).

By introducing the scaling variable

$$x_\tau=L_\tau^{1/\nu}\left(\frac{1}{\lambda}-\frac{1}{\lambda_c}\right), \qquad (18)$$

where

$$L_\tau=\left(\frac{\lambda}{t}\right)^{1/z}, \qquad (19)$$

and $\nu^{-1}=d-\frac{1}{2}\sigma$ and $z=\frac{1}{2}\sigma$ are the critical exponents of the model (Vojta, 1996), the singular part of the free energy, Eq. (16), takes the form of Eq. (1) with

$$X(x_\tau\,|\,d,\sigma)=-\frac{1}{2}x_\tau y_\tau^2 -\frac{k_d}{4\sigma\sqrt{\pi}}\Gamma\left(\frac{d}{\sigma}\right)\Gamma\left(-\frac{d}{\sigma}-\frac{1}{2}\right)y_\tau^{\frac{2d}{\sigma}+1} -\frac{k_d}{\sigma\sqrt{\pi}}\Gamma\left(\frac{d}{\sigma}\right)\left(2y_\tau^2\right)^{\frac{d}{\sigma}+\frac{1}{2}}\sum_{m=1}^{\infty}\frac{K_{\frac{d}{\sigma}+\frac{1}{2}}(my_\tau)}{(my_\tau)^{\frac{d}{\sigma}+\frac{1}{2}}} \qquad (20)$$

in which $y_\tau=L_\tau^z\phi^{1/2}$ is the solution of the spherical field equation

$$x_\tau=-\frac{k_d}{2\sigma\sqrt{\pi}}\Gamma\left(\frac{d}{\sigma}\right)\left|\Gamma\left(\frac{1}{2}-\frac{d}{\sigma}\right)\right|y_\tau^{\frac{2d}{\sigma}-1} +\frac{2k_d}{\sigma\sqrt{\pi}}\Gamma\left(\frac{d}{\sigma}\right)\left(2y_\tau^2\right)^{\frac{d}{\sigma}-\frac{1}{2}}\sum_{m=1}^{\infty}\frac{K_{\frac{d}{\sigma}-\frac{1}{2}}(my_\tau)}{(my_\tau)^{\frac{d}{\sigma}-\frac{1}{2}}}. \qquad (21)$$

At $x_\tau=0$ ($\lambda=\lambda_c$) from Eq. (20) one obtains the "temporal" Casimir amplitude, $\Delta_{\mathrm{Cas}}^t(d,\sigma)$,

$$\Delta_{\mathrm{Cas}}^t(d,\sigma)=-\frac{k_d}{4\sigma\sqrt{\pi}}\Gamma\left(\frac{d}{\sigma}\right)\Gamma\left(-\frac{d}{\sigma}-\frac{1}{2}\right)y_0^{\frac{2d}{\sigma}+1} -\frac{k_d}{\sigma\sqrt{\pi}}\Gamma\left(\frac{d}{\sigma}\right)\left(2y_0^2\right)^{\frac{d}{\sigma}+\frac{1}{2}}\sum_{m=1}^{\infty}\frac{K_{\frac{d}{\sigma}+\frac{1}{2}}(my_0)}{(my_0)^{\frac{d}{\sigma}+\frac{1}{2}}}, \qquad (22)$$

where y_0 is the solution of the corresponding equation for the spherical field, which cannot be solved analytically for an arbitrary reduced dimensionality d/σ. The result given by Eq. (22) has been obtained in (Chamati et al., 2000).

5. THE CRITICAL AMPLITUDE OF THE SPECIFIC HEAT IN A SPECIAL CASE

According to Eq. (11), the critical amplitudes of the specific heat can be prepared in a simple, analytical, closed form in some particular cases where for the "temporal" Casimir amplitude useful analytical results may be obtained.

In the particular case $d=\sigma$ Eq. (22) simplifies considerably. In this case the solution y_0 of Eq. (21) at $x_\tau=0$ is $y_0=2\ln\left[\left(1+\sqrt{5}\right)/2\right]$ (Chamati et al., 1997; Chamati et al., 1998). Setting this value of y_0 in Eq. (22), taking into account that $K_{3/2}(x)=\sqrt{\pi/(2x)}\exp(-x)(1+1/x)$ and using the properties of the polylogarithm functions $Li_p(x)$ (Sachdev, 1993), according to Eq. (11), we obtain after some algebra that the critical amplitude of the specific heat is

$$C_s\left(0\,|\,\sigma\right)=-6\Delta^t_{\text{Cas}}\left(\sigma,\sigma\right)=\frac{96\varsigma\left(3\right)}{5\sigma\left(4\pi\right)^{\sigma/2}\Gamma\left(\sigma/2\right)}, \tag{23}$$

where $\varsigma\left(x\right)$ is the Riemann zeta function. When $\sigma\neq 2$ it is easy to verify that the following general relation

$$\frac{C_s\left(0\,|\,\sigma\right)}{C_s\left(0\,|\,2\right)}=\frac{\Delta^t_{\text{Cas}}\left(\sigma,\sigma\right)}{\Delta^t_{\text{Cas}}\left(2,2\right)}=\frac{8\pi}{\sigma\left(4\pi\right)^{\sigma/2}\Gamma\left(\sigma/2\right)} \tag{24}$$

holds. Let us note that the relation Eq. (24) between the "temporal" Casimir amplitudes have been obtained in (Chamati et al., 2000).

6. CONCLUSIONS

The specific heat of a d-dimensional quantum system is studied close to the quantum critical point in the framework of the theory of FSS.

We have obtained that at $g=g_c$, i.e. in the quantum critical region, when the dynamical critical exponent $z=1$ the Debye law holds.

It is shown that at $T=0$ the critical exponent $\alpha_{\delta g}$, associated with the susceptibility $\chi_{\delta g}$, given by Eq. (4), satisfies the hyperscaling relation.

From the obtained relation between the scaling functions of the specific heat and the free energy density, Eq. (9), we have derived a general relationship between corresponding critical amplitudes, Eq. (11).

In the example of the QSRM for the special case $d=\sigma$ the critical amplitude of the specific heat is derived in a simple, analytical, closed form, Eq. (23).

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