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On the critical specific heat capacity of a classical anharmonic crystal with long-range interaction

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Abstract. The bulk critical specific heat capacity of a classical anharmonic crystal with long-range interaction (decreasing at large distances r as $r^{-d-\sigma}$, where d is the space dimensionality and $0 < \sigma \leq 2$) is studied. An exact analytical expression is obtained at the upper critical dimension $d = 2\sigma$ of the system. This result depends on both the deviation from the critical point and the space dimensionality of the system, while the known asymptotic one depends only on the deviation from the critical point. For real systems (chains, thin layers, *i.e.* films and three-dimensional systems) the exact result and the asymptotic one are graphically presented and compared on the basis of the calculated relative errors. The obtained result holds true in a broader neighborhood of the critical point. The expansion of the critical region is estimated at the three real physical dimensionalities.

1. The model

The considered model describes a structural phase transition of second kind. The Hamiltonian of the model is [1]

$$H = \frac{1}{2}\sum_{\mathbf{r}}\left(\frac{P_{\mathbf{r}}^2}{m} - AQ_{\mathbf{r}}^2\right) + \frac{1}{4}\sum_{\mathbf{r},\,\mathbf{r}'}\varphi(\mathbf{r}-\mathbf{r}')(Q_{\mathbf{r}} - Q_{\mathbf{r}'})^2 + \frac{B}{4N}\left(\sum_{\mathbf{r}} Q_{\mathbf{r}}^2\right)^2, \tag{1}$$

where $P_{\mathbf{r}}$ and $Q_{\mathbf{r}}$ are the operators of displacement and momentum, respectively, of the particle of mass m at site $\mathbf{r}$ of a d-dimensional hypercubic lattice. The parameter $A = \nu_0^2 m > 0$ determines the frequency of a mode which is unstable in the harmonic approximation and the parameter $B > 0$ introduces an anharmonic interaction which is inversely proportional to the particle number N. The harmonic force constants $\varphi(\mathbf{r}-\mathbf{r}')$ which are assumed to decrease at large distances $r = |\mathbf{r}-\mathbf{r}'|$ as $r^{-d-\sigma}$, describe a short-range ($\sigma = 2$) or a long-range ($0 < \sigma < 2$) interaction.

The free energy density of the model (1), obtained by using *approximating Hamiltonian method* is [2, 3]

$$f = \frac{A^2}{B} f_0 = \frac{A^2}{B}\left(\frac{1}{2} I_{t,\lambda}^{d,\sigma}(\bar{\Delta}) - \frac{1}{4}(1+\bar{\Delta})^2\right), \tag{2}$$

where $\bar{\Delta}$ is the solution of the self-consistent equation

$$\frac{dI_{t,\lambda}^{d,\sigma}(\Delta)}{d\Delta} = 1 + \Delta. \tag{3}$$

In the thermodynamic limit $N \to \infty$ the function $I_{t,\lambda}^{d,\sigma}$ is defined by

$$I_{t,\lambda}^{d,\sigma}(\Delta) = 2t \frac{S_d}{(2\pi)^d} \int_0^{x_D} x^{d-1} \ln\left(2\sinh\left(\frac{\lambda}{2t}\sqrt{\Delta + x^\sigma}\right)\right) dx, \tag{4}$$

where $t = T/(4E_0)$ is the dimensionless temperature and $\lambda = \hbar\nu_0/(4E_0)$ is a parameter which switches on the quantum fluctuations, $E_0 = A^2/(4B)$ is the barrier height of the double-well potential in (1), $x_D = 2\pi(d/S_d)^{1/d}$ is the radius of the effective sphere replacing the Brillouin zone and $S_d = 2\pi^{d/2}/\Gamma(d/2)$ (Γ is the Euler gamma function) is the surface of the d-dimensional unit sphere. Setting $\Delta = 0$ into (3) one obtains the critical point $t_c(\lambda)$. In the disordered phase ($t > t_c$), $\bar{\Delta}$ is finite and the susceptibility of the system is $\chi = \bar{\Delta}^{-1}$.

Let us note that the equations (2) and (3) play a central role in the study of the bulk critical behavior of the model, *e.g.* for the specific heat capacity $c(T) \equiv -T\partial^2 f/\partial T^2$ from (3) and (2), we obtain

$$c(t) = -t\frac{\partial^2 f_0}{\partial t^2} = -\frac{t}{2}\left(\frac{\partial^2 I_{t,\lambda}^{d,\sigma}(\bar{\Delta})}{\partial t^2} - \left(\frac{\partial\bar{\Delta}}{\partial t}\right)^2 - (1+\bar{\Delta})\frac{\partial^2\bar{\Delta}}{\partial t^2}\right). \tag{5}$$

This model retains many fundamental properties of the real systems related to the presence of both quantum and classical fluctuations, depending on the temperature T, the quantum parameter λ, the long-range interaction exponent σ and the spatial dimensionality d. For a more complete discussion of the bulk critical behavior and the finite-size properties of the model and its generalizations, see [3] and references therein.

Exact solutions of the self-consistent equation (3), in terms of the Lambert W-function [4], have been obtained in both the quantum and the classical limits at the corresponding upper critical dimensions, $d = 3\sigma/2$ and $d = 2\sigma$, respectively [5,6]. On the basis of the solution at $d = 3\sigma/2$, an exact expressions for the bulk free energy density near the quantum critical point $T = 0$ has been obtained in [7]. The finite-size corrections to the free energy density for the pure quantum version of the model have been studied in [8].

In this paper, using the exact solution of the self-consistent equation (3) in the classical limit ($\lambda \to 0^+$) at the upper critical dimension $d = 2\sigma$ [6], we establish an exact analytical expression for the specific heat capacity of the model in terms of the Lambert W-function. For systems with real physical dimensions (chains, thin layers, *i.e.* films and three-dimensional systems), the obtained exact result is graphically presented and compared with the asymptotic one on the basis of the calculated relative error. We show that the obtained exact result for the specific heat capacity holds true in a broader neighborhood of the critical point. Besides, we give an estimate for the expansion of the critical region at the three real physical dimensionalities.

2. An exact result and its leading asymptotic behavior

For classical systems ($\lambda \to 0^+$) the self-consistent equation (3) gets the form

$$\frac{dU_{d,\sigma}(\Delta)}{d\Delta} = \frac{1}{t}(1+\Delta), \tag{6}$$

where the function U is defined by

$$U_{d,\sigma}(\Delta) = \frac{S_d}{(2\pi)^d}\int_0^{x_D} x^{d-1}\ln(\Delta + x^\sigma)dx. \tag{7}$$

For the critical temperature from (6) at $\Delta = 0$, we obtain

$$t_c = \frac{d-\sigma}{d}\, x_D^\sigma. \tag{8}$$

In the classical limit from (4), taking into account (6), we get

$$\frac{\partial^2 I^{d,\sigma}_{t,0}(\bar{\Delta})}{\partial t^2} = -\frac{2}{t} + \frac{1}{t}(1+\bar{\Delta})\frac{\partial\bar{\Delta}}{\partial t} + \left(\frac{\partial\bar{\Delta}}{\partial t}\right)^2 + (1+\bar{\Delta})\left(\frac{\partial^2\bar{\Delta}}{\partial t^2}\right). \tag{9}$$

Thus, from the last equation and (5), we obtain the following expression for the specific heat capacity of the model (1) in the classical limit

$$c(t) = 1 - \frac{1}{2}(1+\bar{\Delta})\frac{\partial\bar{\Delta}}{\partial t}. \tag{10}$$

Similar result was obtained in the framework of the mean spherical model [3, p.89] which belongs to the same universality class [9].

Since in the disordered phase ($t > t_c$) near the critical point ($t \to t_c^+$) the solution $\bar{\Delta}$ of (6) decreases when t decreases and $\bar{\Delta} = 0$ in the ordered phase ($t < t_c$), then the specific heat capacity keeps its maximum value $c(t) = 1$ for all $t \le t_c$ and the Dulong-Petit low of the classical thermodynamics holds for all $T \le T_c$.

At the upper classical critical dimension ($d = 2\sigma$), near the classical critical point ($t \to t_c^+$), *i.e.* when $\Delta << 1$, the equation (6) can be written in the following form

$$\left(\frac{\Delta}{x_D^\sigma}\right)\ln\left(\frac{\Delta}{x_D^\sigma}\right) - x_D^\sigma\left(\frac{\Delta}{x_D^\sigma}\right) = -\epsilon, \tag{11}$$

where $\epsilon = 1 - t_c/t$ is a measure of the deviation of the critical point. From (8), for the critical temperature in this case, we get $t_c = x_D^\sigma/2$. The exact solution of (11) in terms of the Lambert W-function is [6]

$$\bar{\Delta} = x_D^\sigma \exp[x_D^\sigma + W_{-1}(-\epsilon\, e^{-x_D^\sigma})], \tag{12}$$

where $W_{-1}(x)$ is the real branch of the Lambert W-function on the interval $[-1/e, 0)$, satisfying $W_{-1}(x) \le -1$, as $\lim_{x\to 0^-} W_{-1}(x) = -\infty$ [4]. Thus, in the neighborhood of the classical critical point ($\epsilon \to 0^+$) at the upper classical critical dimension $d = 2\sigma$, from (12) and (10), we get the following exact expression for the specific heat capacity of the model (1)

$$c(\epsilon) = 1 + \frac{1}{1 + W_{-1}(-\epsilon\, e^{-x_D^\sigma})}\left(1 - x_D^\sigma \frac{\epsilon}{W_{-1}(-\epsilon\, e^{-x_D^\sigma})}\right). \tag{13}$$

The last result shows that the specific heat capacity remains finite at $T_c(\epsilon = 0)$ but in this point its graph has a cusp. The obtained expression (13) allow us to find a critical region in which the specific heat decreases n times. For $c(\epsilon) = 1/n$, from (13) neglecting the second term in the brackets, we obtain that the endpoint of this critical region is

$$\epsilon_n = \frac{(2n-1)}{n-1}\, e^{\frac{2n-1}{1-n} + x_D^\sigma}, \qquad n > 1. \tag{14}$$

From (13), using the series in the asymptotic formula of the Lambert W-function [4] and retaining the leading term, we get the following asymptotic behavior of the specific heat capacity

$$c_{appr.} \approx 1 + \frac{1}{\ln\epsilon}. \tag{15}$$

From the other hand, the last result can be obtained from (10) using the known asymptotic behavior [6]

$$\bar{\Delta}_{appr.} \approx -x_D^\sigma \frac{\epsilon}{\ln\epsilon}. \tag{16}$$

Note that the logarithmic correction in (15) was discussed in the framework of the mean spherical model in [3].

From (15), for the endpoint $\epsilon_{n,appr.}$ of a critical region in which the asymptotic specific heat capacity decreases n times, we have

$$\epsilon_{n,appr.} = e^{\frac{n}{1-n}}\,, \qquad n > 1.$$

From this and (14), we get the following relation

$$\epsilon_n = \frac{2n-1}{n-1}\, e^{x_D^\sigma - 1}\epsilon_{n,appr.}\,, \qquad n > 1 \tag{17}$$

which shows that $\epsilon_n > \epsilon_{n,appr.}$ for each $0 < \sigma \leq 2$ and gives an estimate for the expansion of the critical region. Let us note that for all n this expansion increases with σ, *i.e.* with the dimensionality of the system d.

3. Comparison between the exact result and the asymptotic one

It is easy to see from (13) and (15) that the exact result depends on both the deviation from the critical point and the dimensionality of the system, while its leading asymptotic behavior depends only on the deviation from the critical point. For systems with real physical dimensionalities (chains, films and three-dimensional systems), on figure 1 we present the obtained exact and asymptotic results for the specific heat capacity.

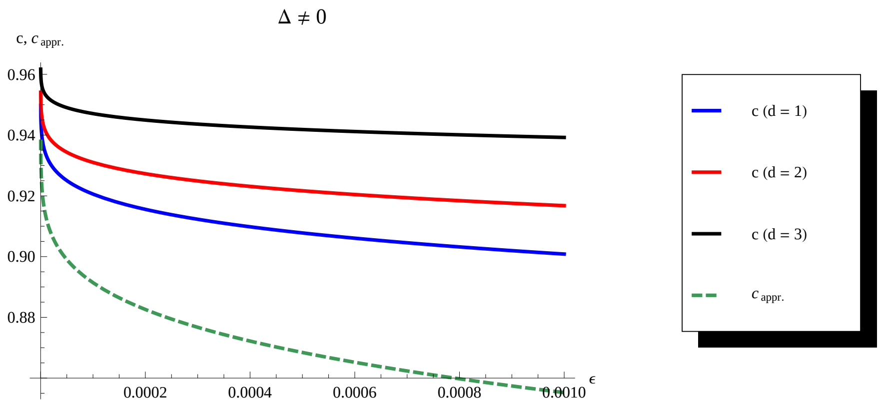

Figure 1. The dependences of the specific heats c and $c_{appr.}$ on the deviation from the critical point ϵ.

For more detailed analysis in the table 1, we give some numerical data for the computed relative errors $|1 - \bar{\Delta}_{appr.}/\bar{\Delta}|$ and $|1 - c_{appr.}/c|$ as functions of the deviation from the critical point and the dimensionality of the system.

Table 1. Percent relative errors [%].

	$\mathbf{d=1}(\sigma=\mathbf{1/2})$		$\mathbf{d=2}(\sigma=\mathbf{1})$		$\mathbf{d=3}(\sigma=\mathbf{3/2})$	
ϵ	$\left\|1-\frac{\bar{\Delta}_{appr.}}{\bar{\Delta}}\right\|$	$\left\|1-\frac{c_{appr.}}{c}\right\|$	$\left\|1-\frac{\bar{\Delta}_{appr.}}{\bar{\Delta}}\right\|$	$\left\|1-\frac{c_{appr.}}{c}\right\|$	$\left\|1-\frac{\bar{\Delta}_{appr.}}{\bar{\Delta}}\right\|$	$\left\|1-\frac{c_{appr.}}{c}\right\|$
1×10^{-7}	29.8	1.2	41.3	1.6	68.2	2.4
1×10^{-6}	33.9	1.6	47.4	2.1	78.9	3.1
1×10^{-5}	39.5	2.1	55.8	2.9	93.8	4.1
1×10^{-4}	47.5	3.1	68.2	4.2	116.0	5.8
1×10^{-3}	60.4	5.0	88.4	6.7	152.8	8.9

4. Conclusions

Using the exact solution (12) of the self-consistent equation, in the neighborhood of the classical critical point at the upper critical dimension of the system, an exact analytical expression for the specific heat capacity (13) is obtained.

It is shown that the exact specific heat capacity depends on both the deviation from the critical point $\epsilon = 1 - t_c/t$ and the long-range interaction exponent σ, *i.e.* of the space dimensionality d of the system. Its leading asymptotic behavior (15), has a logarithmic correction depending only on ϵ which is well known in the theory of the critical phenomena.

For real systems (chains, thin layers, *i.e.* films and three-dimensional systems) the specific heat capacity and its leading asymptotic behavior are graphically presented on figure 1. One can see from the graph that the specific heat capacity increases with the space dimensionality of the system. Moreover, the obtained result (13) holds true in a broader neighborhood of the critical point. The expressions (13) and (15) allow us to estimate the expansion of the critical region as a function of the spatial dimensionality of the system (17). Note that this expansion increases with dimensionality of the system d.

It is easy to see from the table 1 that at each deviation from the critical point and each dimensionality, the relative error for the specific heat capacity is less than the relative error for the inverse susceptibility.

Finally, the exact solution of the self-consistent equation can be used in investigating of the other critical thermodynamical properties of the system, *e.g.* the entropy and others.

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References

[1] Schneider T, Stall E and Beck H 1975 *Physica A* **79** 201
[2] Plakida N M, Radosz A and Tonchev N S 1991 *Phase Transitions* **297** 179
[3] Brankov J G, Danchev D M and Tonchev N S 2000 The Theory of Critical Phenomena in Finite-Size Systems - Scaling and Quantum Effects *Series in Modern Condensed Matter Physics* vol 9 (Singapore: World Scientific) p 1
[4] Corlles R M, Gonnet G H, Hare D E, Jeffrey D J and Knuth D E 1996 *Advances in Comput. Math.* **5** 329
[5] Pisanova E S, Tonchev N S and Kisov Hr T 2009 *AIP Conf. Proc.* **1203** 255
[6] Pisanova E S and Ivanov S I 2013 *Bulgarian Journal of Physics* **40** 159
[7] Pisanova E S and Tonchev N S 2010 *Journal of Physics: Conference Series* **253** 012020
[8] Chamati H 1994 *Physica A* **212** 357
[9] Kadanoff L P 1971 *Proc. Intern. School of Physics "Enrico Fermi"* (New York: Academic Press)