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On the Critical Behavior of the Inverse Susceptibility of a Model of Structural Phase Transitions*

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Abstract. An exactly solvable lattice model describing structural phase transitions in an anharmonic crystal with long-range interaction is considered in the neighborhoods of the quantum and classical critical points at the corresponding upper critical dimensions. In a broader neighborhood of the critical region the inverse susceptibility of the model is exactly calculated in terms of the Lambert W-function and graphically presented as a function of the deviation from the critical point and the upper critical dimension. For quantum and classical systems with real physical dimensions (chains, thin layers and three-dimensional systems) the exact results are compared with the asymptotic ones on the basis of some numerical data for their ratio. Relative errors are also provided.

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1 The Model

In this study, we consider a model which in both bulk and finite-size cases has been exactly studied in a variety of papers (see *e.g.* [1], [2, Chapter 3] and references therein). The Hamiltonian of this model is

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

where $P_{\mathbf{r}}$ and $Q_{\mathbf{r}}$ are operators of displacement and momentum, respectively, of the particle of mass m at site $\mathbf{r}$ of a d-dimensional hypercubic lattice. The parameter $A = \nu_0 m > 0$ determines the frequency of a mode which is unstable in the harmonic approximation. The parameter $B > 0$ introduces into the model 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

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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.

In the thermodynamic limit $N \to \infty$ the inverse susceptibility $\Delta = \chi^{-1}$ of the system satisfies the following self-consistent equation [1, 2]:

$$1 + \Delta = \frac{\lambda}{2} \frac{S_d}{(2\pi)^d} \int_0^{x_D} \frac{x^{d-1}}{\sqrt{\Delta + x^\sigma}} \coth\left(\frac{\lambda}{2t}\sqrt{\Delta + x^\sigma}\right) dx. \qquad (2)$$

In (2), $t = T/(4E_0)$ 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 $S_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface of the d-dimensional unit sphere ($\Gamma(z)$ is the Euler gamma function).

The model (1) describes a phase transition of second kind at the critical temperature $t_c = t_c(\lambda)$ which vanishes at a critical value λ_c of the quantum parameter λ. In real systems, the external pressure or the amount of impurities reduces the critical temperature. At the critical point, the solution of (2) is $\Delta = 0$. In the disordered phase ($t > t_c(\lambda)$) Δ is finite and the susceptibility of the system is $\chi = \Delta^{-1}$.

This paper is a continuation of the exact computation of non-universal characteristics in the upper critical dimensions by applying the Lambert W-function [3], particularly in a broader neighborhood of the critical point. Exact expressions for the inverse susceptibility [4] and the free energy density [5] of the considered model have been obtained near the quantum critical point at the upper quantum critical dimension $d = d_u^q = 3\sigma/2$. In addition to [4], here we obtain an exact analytical expression for the inverse susceptibility of the model near the classical critical point at the upper classical critical dimension $d = d_u^{cl} = 2\sigma$. In both cases, the quantum and classical, the exact inverse susceptibilities and asymptotic ones as functions of the deviation from the critical point and the upper critical dimension are graphically presented and compared on the basis of the calculated relative errors.

Due to the fact that we consider systems with long-range interaction, *i.e.* $0 < \sigma \leq 2$, the upper critical dimension may coincide with one of the three real physical dimensions: (i) For quantum systems $d = 1$ if $\sigma = 2/3$, $d = 2$ if $\sigma = 4/3$ and $d = 3$ if $\sigma = 2$ (the short-range interaction); (ii) For classical systems $d = 1$ if $\sigma = 1/2$, $d = 2$ if $\sigma = 1$ and $d = 3$ if $\sigma = 3/2$.

2 Exact Expressions for Inverse Susceptibility

We shall consider two main possibilities of phase transition: (i) At $t = 0$, controlled by the quantum parameter λ ($\lambda \to \lambda_c^+$); (ii) At $\lambda = 0$, controlled by the temperature t ($t \to t_c^+$). Using the parameters θ and ρ associated with θ

($\rho = 1/2$ at $\theta = \lambda$ – for quantum systems and $\rho = 1$ at $\theta = t$ – for classical systems) near the quantum ($t = 0, \lambda = \lambda_c$) and the classical ($\lambda = 0, t = t_c$) critical points, we can write (2) in a summarised form

$$1 + \Delta = \rho\theta \frac{S_d}{(2\pi)^d} \int_0^{x_D} \frac{x^{d-1}}{(\Delta + x^\sigma)^\rho} dx. \tag{3}$$

The last equation has solution a $\Delta = 0$ at the critical point $\theta = \theta_c = [(d - \rho\sigma)(2\pi)^d]/[\rho x_D^{d-\rho\sigma} S_d]$, where $d > \rho\sigma$. At the upper critical dimension $d = d_u = (\rho + 1)\sigma$ the equation (3) has the form

$$1 + x_D^\sigma \tilde{\Delta} = \theta/[\theta_c(\rho + 1)(1 + \tilde{\Delta})^\rho] F(\rho, 1; \rho + 2; 1/[1 + \tilde{\Delta}]), \tag{4}$$

where $\tilde{\Delta} = \Delta/x_D^\sigma$ is the renormalized inverse susceptibility and $F(\alpha, \beta; \gamma; z)$ is the hypergeometric function.

Now let us consider equation (4) sufficiently close to the critical point $\theta \to \theta_c$, *i.e.* , when $\tilde{\Delta} << 1$. By applying a well known formula for transformation of the hypergeometric function (see formula (15.3.11) in [6]) and retaining the leading terms, including the linear $\tilde{\Delta}$-term, after some algebra, we can write (4) in the following form:

$$\tilde{\Delta} \ln \tilde{\Delta} + a\tilde{\Delta} = -\rho^{-1}\delta\theta \quad \text{with} \quad a = \psi(\rho + 1) - \psi(1) - 1 - x_D^\sigma \rho^{-1}, \tag{5}$$

where $\psi(x) = d[\ln \Gamma(x)]/dx$ is the ψ-function and $\delta\theta = 1 - \theta_c/\theta$ characterizes the deviation from the critical point θ_c. The exact solution of (5) in terms of the Lambert W-function is

$$\tilde{\Delta} = \exp[W_{-1}(-\rho^{-1}\delta\theta e^a) - a]. \tag{6}$$

The choice of the real branch $W_{-1}(x)$ of the W-function among the solutions of (5) corresponds to the fact that at $\theta = \theta_c$ the renormalized inverse susceptibility $\tilde{\Delta}$ must vanish, which takes place due to the property $W_{-1}(x \to 0^-) \to -\infty$ [3]. Using the series for the branch $W_{-1}(x)$ at $x \to 0^-$ [3] and retaining the leading term, from (6) we get the following asymptotic expression:

$$\tilde{\Delta}_{appr.} \approx \rho^{-1}\delta\theta |\ln \delta\theta|^{-1} \tag{7}$$

which is well known in the theory of phase transitions (see *e.g.* [2]). It can be obtained also by an approximate method if the linear $\tilde{\Delta}$-term in (5) is omitted.

Below, subscripts q and cl mean that the inverse susceptibilities are with respect to quantum ($\delta\theta \equiv \delta\lambda$, $\rho = 1/2$ and $d = 3\sigma/2$) and classical ($\delta\theta \equiv \delta t$, $\rho = 1$ and $d = 2\sigma$) systems, respectively: $\Delta^{q(cl)} = x_D^\sigma \tilde{\Delta}^{q(cl)}$ and $\Delta_{appr.}^{q(cl)} = x_D^\sigma \tilde{\Delta}_{appr.}^{q(cl)}$.

The exact inverse susceptibilities Δ^q, Δ^{cl} and the asymptotic ones $\Delta_{appr.}^q, \Delta_{appr.}^{cl}$ as functions of the deviation from the corresponding critical point and the upper critical dimension for quantum and classical systems are graphically presented in Figure 1 and Figure 2, respectively. In both cases, the bigger value corresponds to the asymptotic expression for the inverse susceptibility (see the values of $\Delta^{q(cl)}/\Delta^{q(cl)}_{appr.}$ in Table 1 and Table 2). For more detailed analysis, some numerical data for the ratio $\Delta^{q(cl)}/\Delta^{q(cl)}_{appr.}$ and the relative error $f = |1 - \Delta^{q(cl)}_{appr.}/\Delta^{q(cl)}|$ for quantum and classical systems with real physical dimensions are given in Table 1 and Table 2, respectively.

The behavior of the ratio Δ^q/Δ^{cl} in dependence on the deviation from the corresponding critical point $\delta\theta$ and the upper critical dimension d of the systems is shown in Figure 3.

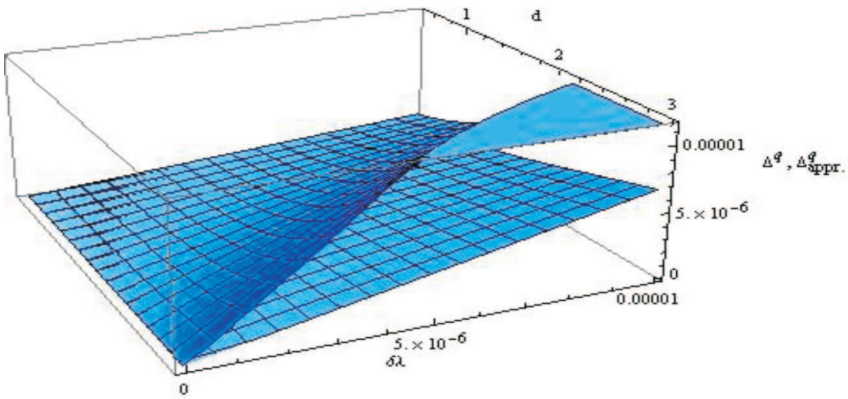

Figure 1: The inverse susceptibility of quantum systems $\Delta^q = \Delta^q(\delta\lambda, d)$ and $\Delta^q_{appr.} = \Delta^q_{appr.}(\delta\lambda, d)$.

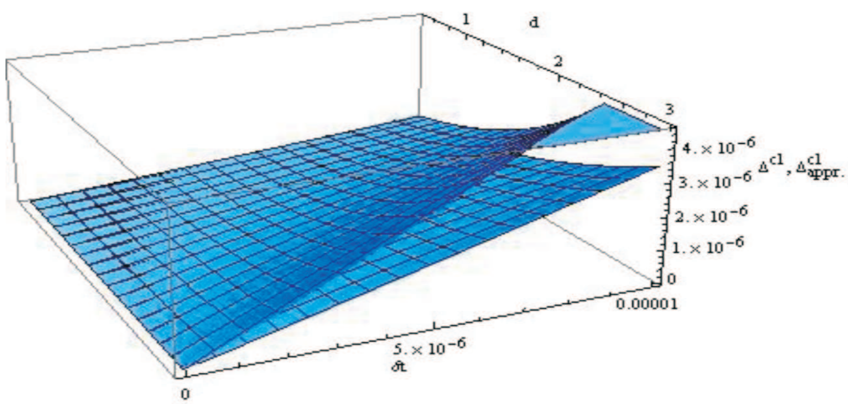

Figure 2: The inverse susceptibilities of classical systems $\Delta^{cl} = \Delta^{cl}(\delta t, d)$ and $\Delta^{cl}_{appr.} = \Delta^{cl}_{appr.}(\delta t, d)$.

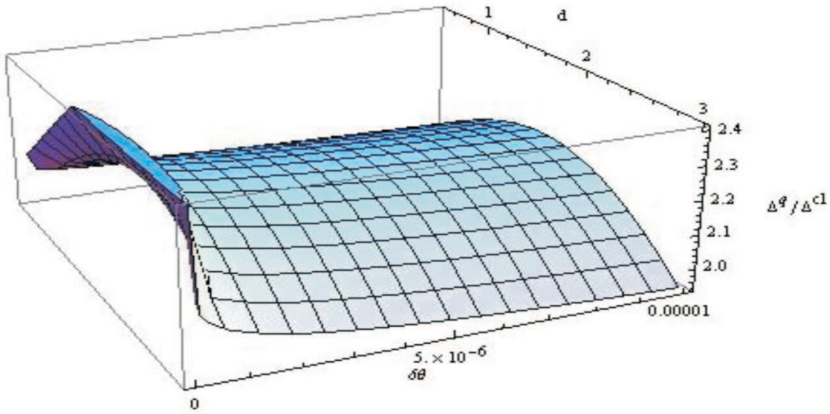

Figure 3: The ratio between the inverse susceptibilities of quantum and classical systems $\Delta^q/\Delta^{cl} = \Delta^q/\Delta^{cl}(\delta\theta, d)$.

Table 1 Numerical data for quantum systems

	$d=1(\sigma=2/3)$		$d=2(\sigma=4/3)$		$d=3(\sigma=2)$	
$\delta\lambda$	$\Delta^q/\Delta^q_{appr.}$	$f[\%]$	$\Delta^q/\Delta^q_{appr.}$	$f[\%]$	$\Delta^q/\Delta^q_{appr.}$	$f[\%]$
1×10^{-11}	0.77	29	0.64	56	0.43	135
1×10^{-10}	0.76	32	0.62	61	0.40	148
1×10^{-9}	0.74	35	0.60	68	0.38	164
1×10^{-8}	0.72	39	0.57	76	0.35	185
1×10^{-7}	0.69	44	0.54	86	0.32	211

Table 2 Numerical data for classical systems

	$d=1(\sigma=1/2)$		$d=2(\sigma=1)$		$d=3(\sigma=3/2)$	
δt	$\Delta^{cl}/\Delta^{cl}_{appr.}$	$f[\%]$	$\Delta^{cl}/\Delta^{cl}_{appr.}$	$f[\%]$	$\Delta^{cl}/\Delta^{cl}_{appr.}$	$f[\%]$
1×10^{-11}	0.83	20	0.78	28	0.69	45
1×10^{-10}	0.82	22	0.77	30	0.67	49
1×10^{-9}	0.80	24	0.75	33	0.65	54
1×10^{-8}	0.79	27	0.73	37	0.62	60
1×10^{-7}	0.77	30	0.71	41	0.59	68

3 Conclusions

The considered model in spite of its high idealization, 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.

In the neighborhoods of the quantum and classical critical points at the corresponding upper critical dimensions exact analytical expressions for the inverse susceptibility $\Delta = x_D^\sigma \tilde{\Delta}$ of the model in terms of the Lambert W-function ($\tilde{\Delta}$ is given by (6)) are obtained. Let as note that the Lambert W-function turns out to be a very effective tool for an exact computation of non-universal characteristics in the upper critical dimensions, especially in a broader neighborhood of the critical point.

One can see from Figure 1 and Figure 2 and also from Table 1 and Table 2 that the asymptotic solutions for the inverse susceptibility are applicable for low dimensional quantum and classical systems, sufficiently close to the critical point. For classical systems the dimensionality and the deviation from the critical point may adopt higher values.

On the other hand Figure 3 shows that for all $\delta\theta$ and d the values of Δ^q are more than two times greater than the values of Δ^{cl}. Besides, for all $\delta\theta$ the ratio Δ^q/Δ^{cl} has maximum at $d = 2$ and increases rapidly sufficiently close to the critical point. But it is important to note that for each fixed value of the upper critical dimension d the long-range interaction exponent σ is different for quantum ($\sigma = 2d/3$) and classical ($\sigma = d/2$) systems.

Finally, this treatment by using the Lambert W-function, can be applied to a wide class of models with logarithmic behavior at the upper critical dimensions (*e.g.* directly to the quantum spherical model [2]).

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