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On the role of the quantum fluctuations in a model of an anharmonic crystal

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An exactly solvable model of an anharmonic crystal, with developed classical and quantum fluctuations depending on the temperature *T*, the quantum parameter λ, the long-range interaction exponent σ and the spatial dimension d is studied below the lower quantum critical dimension. The equation for the inverse susceptibility is analyzed in the low-temperature regime (λ is arbitrary) and in the regime of a small quantum parameter (T is arbitrary) excluding the range around $T = \lambda = 0$. It is shown that in the absence of a phase transition in the system, the quantum fluctuations have a stronger impact on the susceptibility of the classical system, in comparison to the impact of the classical (or thermodynamic) fluctuations on the pure quantum system.

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1. Introduction

The quantum critical regime (i. e. a regime with developed quantum fluctuations) takes place near the zero temperature critical point [1, 2]. In order for such a regime to be attained, one needs to have parameters which can reduce the critical temperature T_c. In real systems, these are the external pressure or the amount of impurity doping [1, 2]. In the low-temperature regime, one can formally consider $1/T$ as an additional finite-size direction of the system considered. This fact provides a useful interpretation of quantum effects as finite-size effects [2].

Exactly solvable models have been used for testing various hypotheses and approximations in the theory of the critical phenomena. For example, a rigorous study of the effect of quantum fluctuations has been given in the framework of a model with the usual single-particle anharmonic interaction (see Chapter 3 in ref. [2] and references therein).

A model system of this type is the exactly solvable model with reduced long-range anharmonic interaction considered in this study. The critical temperature T_c vanishes at a critical value λ_c of the quantum parameter λ (for a review of the model and its generalizations see [2] and references therein). The model considered here retains the most essential feature of real systems, i.e. the dependence of the character of the critical fluctuations (classical and quantum) on the space dimensionality. It yields a conspicuous possibility to investigate in an exact manner the interplay of quantum and classical fluctuations, in dependence on the dimensionality d, the long-range interaction exponent σ and the geometry of the system.

The critical behaviour of the models of this type was studied in refs. [3 -7] in the context of distortive structural phase transitions with a single defect [3], structural phase transitions [4], ferroelectric phase transitions [5], magnetic systems with disorder [6, 7]. The critical exponents on the whole phase diagram, including two multi-critical points (quantum and classical), were calculated in [4].

The aim of this study is to investigate the behaviour of the model with long-range anharmonic interactions, as considered in [4] in the low-temperature regime and in the regime of small quantum parameter, when there is no phase transition in the system (for $d < d_l^q$, where $d_l^q = \sigma/2$ is the lower quantum critical dimension). The reported results complement previous studies [4 - 7] of the competition between quantum and classical fluctuations.

2. The model

The Hamiltonian of the model is [2]

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

Here, $Q_{\mathbf{r}}$ and $P_{\mathbf{r}}$ are the operators of displacement and momentum, respectively, of a particle of mass m at site $\mathbf{r}$ on a d-dimensional hypercubic lattice $\Lambda = L^d$ with periodic boundary conditions. The parameter $A = \nu_0 m > 0$ determines the frequency of the mode which is unstable in the harmonic approximation, and the parameter $B > 0$ introduces into the model an anharmonic interaction, which is inversely proportional to the particle number $N = L^d$. 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.

In the thermodynamic limit $N \to \infty$, the wavelength-dependent inverse susceptibility $\Delta = \chi^{-1}$ of the approximated system obeys the following self-consistency equation [2, 4]

$$1+\Delta = \frac{t}{(2\pi)^d} I(\Delta), \tag{2}$$

where

$$I(\Delta) = \frac{\lambda}{2t}\int_{-\pi}^{\pi}\ldots\int_{-\pi}^{\pi} d^d q \frac{1}{\sqrt{\Delta+|q|^\sigma}} \coth\left(\frac{\lambda}{2t}\sqrt{\Delta+|q|^\sigma}\right) \tag{3}$$

$$= S_d \sum_{m=-\infty}^{\infty}\int_0^{x_D} \frac{x^{d-1}}{\Delta + x^\sigma + bm^2}dx, \tag{4}$$

and $b = 4\pi^2 t^2/\lambda^2$. Here $t = T/4E_0$ 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). Note that quantum effects are important (λ is large), not only at large zero-point energy $\hbar\nu_0$ but also at small depths of E_0. In Eq. (4) $x_D = 2\pi(d/S_d)^{1/d}$ is the effective radius of the sphericalyzed Brillouin zone and $S_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface of the d-dimensional unit sphere.

3. Low-temperature and small λ-corrections in the self-consistency equation

To obtain the low-temperature corrections to the $t=0$ behavior and the small λ-corrections to the $\lambda = 0$ behavior of the model (1), when in the system there is no phase transition, one can use the technique proposed in [8, 9] for studying finite-size scaling in anisotropic systems. This analytical technique is based on some useful properties of the generalized Mittag-Leffler functions (see e. g. [2, 8-11]).

First, with the help of the identity [8]

$$\int_0^\infty \frac{p^{\alpha-1}}{t+p^\eta+q^\tau}dp = \frac{\Gamma\left(1-\frac{\alpha}{\eta}\right)\Gamma\left(\frac{\alpha}{\eta}\right)}{\eta}\cdot\frac{1}{\left(t+q^\tau\right)^{1-\frac{\alpha}{\eta}}},$$

$$\eta>\alpha>0, \tag{5}$$

where $\Gamma(x.)$ is the Euler gamma function, in both the low-temperature $(t\to+0)$ and small quantum parameter $(\lambda\to+0)$ regimes, for Eq. (4) we obtain the result

$$I(\Delta) \approx C_{d,\gamma} b^{-\gamma}\sum_{m=-\infty}^{\infty}\frac{1}{\left(\Delta/b+m^2\right)^\gamma}, \quad 0<\gamma<1, \tag{6}$$

where

$$C_{d,\gamma} = \frac{S_d\Gamma(2-\gamma)\Gamma(\gamma)}{d}, \text{ and } \gamma = 1-\frac{d}{\sigma}. \tag{7}$$

The summation in Eq. (6) can be evaluated [8, 9] in terms of the generalized Mittag-Leffler function $E^\gamma_{\alpha,\alpha\gamma}(z)$, taking into account the identity

$$\frac{1}{\left(\lambda_V + y^\alpha\right)^\gamma} = \int_0^\infty e^{-yt} t^{\alpha\gamma-1} E^\gamma_{\alpha,\alpha\gamma}\left(-\lambda_V t^\alpha\right)dt. \tag{8}$$

If one chooses $y = m^2$, $\lambda_V = \Delta/b$ and $\alpha = 1$ the required result for $0<\gamma<1$ is

$$I(\Delta)\approx C_{d,\gamma}b^{-\gamma}\int_0^\infty x^{\gamma-1}E^\gamma_{1,\gamma}\left(-\frac{\Delta}{b}x\right)\Theta(x)dx, \tag{9}$$

where the notation

$$\Theta(x) = \sum_{m=-\infty}^{\infty} e^{-m^2 x}, \tag{10}$$

has been introduced.

Now let us represent the right-hand side of Eq. (9) as a sum of three terms, $I(\Delta)\approx K_1+K_2+K_3$.

The first one is given by

$$K_1 = C_{d,\gamma}b^{-\gamma}\int_0^\infty x^{\gamma-1}E^\gamma_{1,\gamma}\left(-\frac{\Delta}{b}x\right)\left[\Theta(x)-1-\sqrt{\frac{\pi}{x}}\right]dx$$

$$= C_{d,\gamma}(2\pi)^{2\gamma}b^{-\gamma}F^\gamma_{1,2}\left((2\pi)^2\frac{\Delta}{b}\right), \tag{11}$$

where the introduced universal finite-size scaling function in [8, 9] of the form

$$F^\gamma_{1,2}(y) = \frac{1}{(2\pi)^{2\gamma}}\int_0^\infty x^{\gamma-1}E^\gamma_{1,\gamma}\left(-\frac{xy}{(2\pi)^2}\right)$$

$$\times\left[\Theta(x)-1-\sqrt{\frac{\pi}{x}}\right]dx \tag{12}$$

is used.

The second term is given by

$$K_2 = C_{d,\gamma} b^{-\gamma} \int_0^\infty x^{\gamma-1} E_{1,\gamma}^{\gamma}\left(-\frac{\Delta}{b}x\right)dx = C_{d,\gamma}\Delta^{-\gamma} . \quad (13)$$

In obtaining Eq. (13), we have taken into account the identity [8, 9]

$$\int_0^\infty x^{\gamma\rho-1} E_{\rho,\gamma\rho}^{\gamma}\left(-x^{\rho}\right)dx = 1, \qquad \rho > 0 . \quad (14)$$

The third term is of the form

$$K_3 = C_{d,\gamma} b^{-\gamma} \int_0^\infty x^{\gamma-1} E_{1,\gamma}^{\gamma}\left(-\frac{\Delta}{b}x\right)\sqrt{\frac{\pi}{x}}dx$$
$$= C_{d,\gamma} \mathrm{B}\left(\frac{1}{2},\gamma-\frac{1}{2}\right) b^{-1/2}\Delta^{1/2-\gamma}, \quad \gamma > \frac{1}{2}, \quad (15)$$

where $\mathrm{B}(x,y)$ is the Euler beta function. Equation (15) is obtained by using the elementary representation

$$\sqrt{\frac{\pi}{x}} = \int_0^\infty k^{-1/2} e^{-kx} dk . \quad (16)$$

Collecting together the results of Eqs. (11), (13) and (15) for Eq. (2) in the low-temperature regime $(t \to +0)$ and in the regime of a small quantum parameter $(\lambda \to +0)$, for $1 > \gamma > 1/2$, we obtain:

$$1+\Delta = \frac{C_{d,\gamma}}{(2\pi)^d} \cdot \frac{\lambda^{2\gamma}}{t^{2\gamma-1}}$$
$$\times\left[\frac{\mathrm{B}\left(\frac{1}{2},\gamma-\frac{1}{2}\right)}{2\pi} y^{\frac{1}{2}-\gamma} + F_{1,2}^{\gamma}(y) + y^{-\gamma}\right], \quad (17)$$

where the variable $y = \Delta\lambda^2/t^2$ is introduced.

Equation (17) can be solved only numerically, however some information about the competition between classical and quantum fluctuations can be obtained in the limiting regimes $y >> 1$ and $y << 1$.

The low-temperature corrections to the $t = 0$ behaviour and the small λ-corrections to the $\lambda = 0$ behaviour can be extracted from the asymptotic form of the functions $F_{1,2}^{\gamma}(y)$ at large arguments $y >> 1$ and at small arguments $y << 1$, respectively.

For $y >> 1$, corresponding to the low-temperature regime, using the result for the asymptotic expansion of the finite-size scaling function [8, 9]

$$F_{1,2}^{\gamma}(y) \approx -y^{-\gamma} + \left[\frac{1}{2^{\gamma}\Gamma(\gamma)}\right] y^{-\frac{\gamma}{2}} e^{-\sqrt{y}}, \quad (18)$$

in the case $1/2 < \gamma < 1$, we obtain

$$1+\Delta \approx \frac{C_{d,\gamma}}{(2\pi)^{d+1}} \mathrm{B}\left(\frac{1}{2},\gamma-\frac{1}{2}\right)\lambda\Delta^{\frac{1}{2}-\gamma}$$
$$+\frac{C_{d,\gamma}}{(2\pi)^d}\left[\frac{1}{2^{\gamma}\Gamma(\gamma)}\right]\frac{\lambda^{\gamma}}{t^{\gamma-1}}\Delta^{-\frac{\gamma}{2}} e^{-\frac{\lambda}{t}\sqrt{\Delta}}, \quad (19)$$

that reflects the exponential decay of the low-temperature corrections to the pure quantum ($t = 0$) behaviour of Δ.

For $y << 1$, corresponding to the regime of a small quantum parameter, in the case $1/2 < \gamma < 1$, we get

$$1+\Delta \approx \frac{C_{d,\gamma}}{(2\pi)^d} t\Delta^{-\gamma} + \frac{C_{d,\gamma}}{(2\pi)^{d+1}} \mathrm{B}\left(\frac{1}{2},\gamma-\frac{1}{2}\right)\lambda\Delta^{\frac{1}{2}-\gamma}$$
$$+\frac{C_{d,\gamma}}{(2\pi)}\frac{\lambda^{2\gamma}}{t^{2\gamma-1}} F_{1,2}^{\gamma}(0). \quad (20)$$

The coefficient $F_{1,2}^{\gamma}(0)$ can be evaluated analytically as well as numerically for different values of the free parameter γ $(1/2 < \gamma < 1)$ - see e.g. [12]. In this case, the small λ-contributions to the pure classical ($\lambda = 0$) behaviour of Δ decay algebraically as powers of λ.

4. Conclusions

In the present study we are interested in the forms of the low-temperature corrections to the pure quantum ($t = 0$) behaviour and the small λ-corrections to the pure classical ($\lambda = 0$) behaviour in a model of an anharmonic crystal, commonly used in the theory of phase transitions [2 - 7]. We analyze equation (2) for the inverse susceptibility of the model Eq. (1), when in the system there is no phase transition (below the lower quantum critical dimension, $d < \sigma/2$ or $1/2 < \gamma < 1$).

For this objective, the analytical technique of calculation developed in ref. [8] for the investigation of the finite-size effects in anisotropic systems is utilized. For the equation for the inverse susceptibility (2) in the low-temperature regime and in the regime of small quantum parameter, we obtain respectively Eq. (19) and Eq. (20), which are valid for $d/\sigma < 1/2$ ($1/2 < \gamma < 1$).

As one can see, while the low-temperature correction governed by the second term in the right-hand side of Eq. (19) is exponential in form, the small λ-corrections described by the last two terms in the right-hand side of Eq. (20) are algebraic in form, as powers of λ.

In the considered model, the temperature $t \neq 0$ switches on the classical (or thermodynamic) fluctuations, while the parameter $\lambda \neq 0$ switches on the quantum fluctuations. In the absence of a phase transition in the system, quantum fluctuations have a stronger impact on the susceptibility of the classical system in comparison with the impact of the thermodynamic fluctuations on the pure quantum system. Let us recall that in the case of a phase transition, the influences of both types of fluctuation on the critical behavior are related through the dimensional crossover rule, see [2, 4].

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