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THE ANHARMONIC OSCILLATOR AND DOROCZY-TSALLIS STATISTICS IN THE LOW TEMPERATURE LIMIT

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By allowing for quartic corrections to the Hamiltonian of the harmonic oscillator we study the effect that these corrections have on the thermal energy of an anharmonic oscillator within the context of Doroczy-Tsallis statistics in the low temperature limit.

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1. Introduction

The great progress achieved in the science of statistical physics came about because the systems studied did not admit long range interactions, and the collisions between particles did not leave any memory effects [1,2]. Thus the transition from quantum statistical mechanics to the classical Boltzmann-Gibbs approach can be understood in a way wherein both the exclusion principle and the classical distinguishable nature of particles have a statistical meaning that is simple, and the theory fits the experimental data [3,4]. However, when long-range interactions are present and a non-Markovian memory exists for particle collisions, the principles of statistical mechanics must be re-thought [5]. Situations in both condensed matter physics and in the large-scale scale structure of the universe demand a new approach to statistical mechanics to accommodate the multi-fractral structure brought about by non-Markovian memory effects [6–8]. Motivated by studies in multi-fractrals, Tsallis [5] introduced a non-extensive form for the entropy that accommodates the self similarity for systems with long-range interactions and non-Markovian memory [9]. Applications of the non-extensive statistics of Tsallis to the solar plasma have provided a cutoff for the high energy tail of the Maxwell-Boltzmann distribution leading to the production of solar neutrinos in accord with experimental findings [10–12]. Other applications of the Tsallis statistics include studies of a generalized H theorem [13–15], the fluctuation-dissipation theorem [16], the Langevin and Fokker-Planck equation [17], the classical equipartition theorem [18], the Ising chain

[19,20], paramagnetic systems [21] and the Planck radiation law [22]. Limits on the non-extensive statistics parameter can be set by studying how the non-extensive statistics affects the primordial helium abundance in cosmology [23]. In a previous note, we studied the effect that the non-extensive statistics of Tsallis had on the Debye theory of heat capacities [24]. In that study, we had to resort to an approximate treatment to calculate the chemical potential and occupation numbers of the various states, while in the present note we improve on this treatment by calculating the chemical potential at low temperature by summing over the ground state and the first excited state which will have the dominant occupation numbers at low temperature. Also, in that study we applied the q statistics of Doroczy-Tsallis to a bosonic oscillator, which might suggest an inconsistency in that Abe [25] and Tsallis [26] explicitly related the q statistics to the q deformed commutation relations. However, a generalized q statistics can be thought of as independent of the bosonic, fermionic, or intermediate statistics of the particles involved (suggested by commutation relations) and can be applied to the energy levels of a system exclusively. This is essentially the ingredient involved in the first form of Tsallis statistics discussed in Ref. 9. In this approach, the statistics of particles discussed is put in at another stage. The discussion of the q expectation value involves lumping together the q form of the entropy and the deformed commutation relations. We do not use this approach, but rather apply the q (Tsallis) modified entropy with the conventional form of the expectation value for the energy. Thus, by using the usual form for the expectation value, we do not engage in an investigation of q deformed commutation relations, in our approach level occupation numbers emerge solely from a variational principle for the entropy along with the constraints on energy and total number of particles. Which approach in Ref. 9 is correct can only be decided by experiment. We also add an anharmonic term to the Hamiltonian of the harmonic oscillator and show that the low temperature limit is calculable, but the high temperature limit gives rise to complicated expressions for the chemical potential in terms of parabolic cylinder functions. By just studying the ground state and the first excited state, we recover the formula for the Einstein heat capacity [27] at low temperatures with the absence of the anharmonic term. We then discuss a modification of the Debye theory for low temperatures when the anharmonic term is present for the lattice vibrations and Tsallis statistics is the relevant statistics for the modes of the lattice vibrations. Finally, we point out that the inclusion of an anharmonic term might serve to describe the non-linear effects of the electromagnetic field at high temperatures [28] when the modes of the electromagnetic field exhibit a multi-fractral structure. Such a situation would be realized in the very early universe [29] when the fields are strong enough so that non-linear effects modify the equations of electromagnetism.

2. *The anharmonic oscillator at low temperatures and Doroczy-Tsallis statistics*

In Ref. 24, we discussed a perturbative approach to Doroczy-Tsallis statistics by varying the expression for the entropy (N_i is the occupation number of state i

and q is the non-extensive parameter)

$$S = \frac{Nk}{q-1} \left(\sum \frac{N_i}{N} - \sum \left(\frac{N_i}{N} \right)^q \right) . \tag{2.1}$$

along with the constraints

$$\sum N_i = const \qquad \sum_i N_i \epsilon_i = const \, , \tag{2.2}$$

to yield

$$N_i = \frac{N}{q^{1/(q-1)}} \ \exp \left(\frac{1}{q-1} \ln \left(1 + \frac{(\mu - \epsilon_i)(q-1)}{\tau} \right) \right) . \tag{2.3}$$

After expanding $\mu = \mu_0 + \alpha\mu_1 + \alpha^2\mu_2$, where $\alpha = q - 1$, we find the following expressions for μ_0, μ_1 and N_i (in terms of α) ($\tau = kT$, k is the Boltzmann constant and T the absolute temperature)

$$\mathrm{e}^{\mu_0/\tau} = \frac{\mathrm{e}}{\sum \mathrm{e}^{-\epsilon_i/\tau}} \, , \tag{2.4}$$

$$\mu_1 = -\frac{\tau}{2} + \frac{1}{2\tau} \ \frac{\sum (\mu_0 - \epsilon_i)^2 \mathrm{e}^{(\mu_0-\epsilon_i)/\tau}}{\sum \mathrm{e}^{(\mu_0-\epsilon_i)/\tau}} \, , \tag{2.5}$$

$$N_i = N\mathrm{e}^{-1} \ \mathrm{e}^{(\mu_0-\epsilon_i)/\tau} \left[1 + \alpha \left(\frac{1}{2} + \frac{\mu_1}{\tau} - \frac{(\mu_0 - \epsilon_i)^2}{2\tau^2} \right) \right] . \tag{2.6}$$

To calculate the average thermal energy of a single particle, we have

$$\langle \epsilon \rangle = \frac{\sum \epsilon_i N_i}{N} = \sum \mathrm{e}^{-1} \ \epsilon_i \ \mathrm{e}^{(\mu_0-\epsilon_i)/\tau} \tag{2.7}$$

$$+\alpha \mathrm{e}^{-1} \left[\frac{\left(\sum \epsilon_i \mathrm{e}^{(\mu_0-\epsilon_i)/\tau}\right) \sum (\mu_0 - \epsilon_i)^2 \mathrm{e}^{(\mu_0-\epsilon_i)/\tau}}{2\tau^2 \sum \mathrm{e}^{(\mu_0-\epsilon_i)/\tau}} - \frac{1}{2\tau^2} \sum \epsilon_i (\mu_0 - \epsilon_i)^2 \mathrm{e}^{(\mu_0-\epsilon_i)/\tau} \right] .$$

Eq. (2.7) is the result of substituting Eq. (2.5) into Eq. (2.6) and then averaging over all states. In Ref. 24, we calculated $\mu_1 = -\tau/2$ and $\mu_0 = \hbar\omega/2$ for $\hbar\omega/\tau \gg 1$ (low T). However, these results do not fully take into account the states above the ground state in approximating μ_0 and μ_1. In the present study, we develop a more precise calculation of μ_0 and μ_1 at low T when the Hamiltonian also contains an anharmonic term proportional to x^4. For the energy levels of the anharmonic oscillator described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{kx^2}{2} + \bar{k}x^4 \, ,$$

we find from time independent perturbation theory ($\beta^2 = m\omega_0/\hbar$)

$$E = \left(n + \frac{1}{2}\right)\hbar\omega + \frac{3\bar{k}}{4\beta^4}(2n(n+1)+1) \tag{2.8}$$

(see Ref. [30]). Eq. (2.8) can be written as

$$E_n = a + bn + cn^2\,, \tag{2.9}$$

with $a = \hbar\omega/2 + 3\bar{k}/(4\beta^4)$, $b = \hbar\omega + 3\bar{k}/(4\beta^4)$ and $c = 3\bar{k}/(2\beta^4)$. At very low T ($\hbar\omega/\tau \gg 1$), we may approximate Eq. (2.4) and Eq. (2.7) by summing over the ground state and the first excited state. Then Eq. (2.4) becomes

$$\mathrm{e}^{\mu_0/\tau} = \frac{\mathrm{e}^{1+a/\tau}}{1 + \mathrm{e}^{-(b+c)/\tau}}\,. \tag{2.10}$$

From Eq. (2.9), $\epsilon_0 = a$ and $\epsilon_1 = a + b + c$, and Eq. (2.10) becomes

$$\mu_0 = \tau\left(1 + \frac{a}{\tau}\right) - \tau\ln\left(1 + \mathrm{e}^{-(b+c)/\tau}\right)\,,$$

and finally,

$$\mu_0 = a + \tau - \tau\mathrm{e}^{-(b+c)/\tau} \qquad \text{for} \qquad (b+c)/\tau \gg 1\,. \tag{2.11}$$

From Eq. (2.7), we find, after a long calculation upon summing over the ground state and first excited state while keeping powers of $\mathrm{e}^{-(b+c)/\tau}$ up to the first order, the following expression for the average energy of an anharmonic oscillator

$$\langle\epsilon\rangle = a + (b+c)\mathrm{e}^{-(b+c)/\tau} + \frac{\alpha}{2\tau^2}(2\tau(b+c)^2 - (b+c)^3)\mathrm{e}^{-(b+c)/\tau}\,. \tag{2.12}$$

In Eq. (2.12), if we set the anharmonic term equal to 0 ($c = 0$), and we pass to the Boltzmann limit of Tsallis statistics ($\alpha = 0$), we have $\langle\epsilon\rangle = a + b\mathrm{e}^{-b/\tau}$. For $3N$ oscillators, we have $U = 3N\hbar\omega\mathrm{e}^{-\hbar\omega/(kT)}$ (after subtracting off the vacuum energy) and

$$C_v = \left(\frac{\partial U}{\partial T}\right)_v = 3Nk\left(\frac{\hbar\omega}{kT}\right)^2\mathrm{e}^{-\hbar\omega/(kT)}\,. \tag{2.13}$$

Equation (2.13) is just the Einstein value of the heat capacity at low temperatures [27]. To derive the corrections to the Debye formula at low temperatures, we rewrite Eq. (2.12) as

$$\langle\epsilon\rangle = -\left(\frac{\hbar\omega}{2} + \frac{\hbar\omega}{\mathrm{e}^{\hbar\omega/\tau}}\right) \tag{2.14}$$

$$+ \left(a + (b+c)\mathrm{e}^{-(b+c)/\tau} + \frac{\alpha}{2\tau^2}(2\tau(b+c)^2 - (b+c)^3)\right) + \frac{\hbar\omega}{2} + \frac{\hbar\omega}{\mathrm{e}^{\hbar\omega/\tau}}\,.$$

The number of modes of phonons between ω and $\omega+\mathrm{d}\omega$ in a solid at low temperature is $3\omega^2/(2\pi^2 V_0^3)\mathrm{d}\omega$ (V_0 is the speed of sound in solid). Neglecting the vacuum energy in a term, the total energy is

$$U = \int_0^{\omega_M} \frac{\hbar\omega}{\mathrm{e}^{\hbar\omega/\tau - 1}} \frac{3\omega^2}{2\pi^2 V_0^3}\mathrm{d}\omega + \int_0^{\omega_M} \left((b+c)\mathrm{e}^{-(b+c)/\tau} - \frac{\hbar\omega}{\mathrm{e}^{\hbar\omega/\tau} - 1} \right) \frac{3\omega^2}{2\pi^2 V_0^3}\mathrm{d}\omega \quad (2.15)$$

$$+ \int_0^{\omega_M} \frac{\alpha}{2\tau^2} \left(2\tau(b+c)^2 - (b+c)^3 \right) \mathrm{e}^{-(b+c)/\tau} \frac{3\omega^2}{2\pi^2 V_0^3}\mathrm{d}\omega \,.$$

Equation (2.15) can be written as

$$U = C_D T^4 + \left(C_1 T^4 \mathrm{e}^{-3\bar{k}/(\beta^4 kT)} + C_2 T^3 \mathrm{e}^{-3\bar{k}/(\beta^4 kT)} - C_D T^4 \right) \quad (2.16)$$

$$+\alpha[D_1 T^4 + D_2 T^3 + D_3 T^2 - E_1 T^4 - E_2 T^3 - E_3 T^2 - E_4 T]\mathrm{e}^{-3\bar{k}/(\beta^4 kT)} \,.$$

In Eq. (2.16)

$$C_1 = \left(\frac{k^4}{\hbar^3}\right) \frac{3}{2\pi^2 V_0^3} \int_0^\infty x^3 \mathrm{e}^{-x}\mathrm{d}x \,, \qquad D_1 = \left(\frac{k^4}{\hbar^3}\right) \frac{3}{2\pi^2 V_0^3} \int_0^\infty x^4 \mathrm{e}^{-x}\mathrm{d}x \,,$$

$$E_1 = \frac{1}{2}\left(\frac{k^4}{\hbar^3}\right) \frac{3}{2\pi^2 V_0^3} \int_0^\infty x^5 \mathrm{e}^{-x}\mathrm{d}x \,, \qquad C_D = \frac{3k^4}{2\pi^2 \hbar^3 V_0^3}\left(\frac{\pi^4}{15}\right) \,,$$

$$C_2 = \frac{9}{2}\frac{1}{2\pi^2 V_0^3}\left(\frac{\bar{k}}{\beta^4}\right)\left(\frac{k}{\hbar}\right)^3 \int x^2 \mathrm{e}^{-x}\mathrm{d}x \,, \quad (2.17)$$

$$D_2 = \frac{3}{2\pi^2 V_0^3}\left(\frac{6\bar{k}}{\beta^4}\right)\left(\frac{k}{\hbar}\right)^3 \int x^3 \mathrm{e}^{-x}\mathrm{d}x \,,$$

$$D_3 = \frac{3}{2\pi^2 V_0^3}\left(\frac{3\bar{k}}{\beta^4}\right)^2\left(\frac{k^2}{\hbar^3}\right) \int x^2 \mathrm{e}^{-x}\mathrm{d}x \,,$$

$$E_2 = \frac{3}{2\pi^2 V_0^3}\left(\frac{3\bar{k}}{\beta^4}\right)\frac{3}{2}\left(\frac{k^3}{\hbar^5}\right) \int x^4 \mathrm{e}^{-x}\mathrm{d}x \,,$$

$$E_3 = \frac{3}{2\pi^2 V_0^3}\left(\frac{3\bar{k}}{\beta^4}\right)^2\frac{3}{2}\left(\frac{k^2}{\hbar^4}\right) \int x^3 \mathrm{e}^{-x}\mathrm{d}x \,,$$

$$E_4 = \frac{3}{2\pi^2 V_0^3}\left(\frac{3\bar{k}}{\beta^4}\right)^3\left(\frac{k}{\hbar^3}\right) \int x^2 \mathrm{e}^{-x}\mathrm{d}x \,,$$

(C_D is constant in Debye formula). In Eq. (2.16), we have redefined the range on $x = \hbar\omega/\tau$ from 0 to $\hbar\omega_{\rm M}/\tau$, where $\omega_{\rm M} = (3N\ 2\pi^2 V_0^3)^{1/3}$ is the maximum frequency of phonon modes, and we have extended it from 0 to ∞ at low $\tau = kT$. In Eq. (2.16), if the anharmonic term vanishes ($\bar{k} = 0$), then the heat capacity at low T will have corrections of orders T^3, T^2, T and T^0 after differentiating Eq. (2.17) ($C_V = \partial U/\partial T$). The factor $\exp(-3\bar{k}/(\beta^4 kT))$ in Eq. (2.16) is purely due to the anharmonic term and would be significant at low T. Equation (2.12) would also apply to the black body spectrum at low T if the anharmonic term is set equal to 0. In that case, Eq. (2.12) reads

$$\langle\epsilon\rangle = a + \hbar\omega {\rm e}^{-\hbar\omega/\tau} + \frac{\alpha}{2\tau^2}\left(2\tau(\hbar\omega)^2 - (\hbar\omega)^3\right){\rm e}^{-\hbar\omega/\tau}\,. \tag{2.18}$$

Subtracting off the vacuum term (a), we have ($\tau = kT$)

$$\langle\epsilon\rangle = \hbar\omega {\rm e}^{-\hbar\omega/\tau} + \frac{\alpha}{2\tau^2}\left(\frac{\alpha}{kT} - \frac{\alpha(\hbar\omega)^3}{(kT)^2}\right){\rm e}^{-\hbar\omega/\tau}\,.$$

For the energy per unit frequency range we have

$${\rm d}U(\nu) = \left(h\nu + \alpha\left(\frac{(h\nu)^2}{kT} - \frac{(h\nu)^3}{2(kT)^2}\right)\right){\rm e}^{-h\nu/kT}\frac{8\pi\nu^2{\rm d}\nu}{C^3}\,. \tag{2.19}$$

If the correction term is to be of the same order as the CMB anisotropy, we have from Eq. (2.19) $\alpha \leq 10^{-5}$ [31] since at $T = 3$ K, $h\nu = kT$ for microwaves ($\lambda \simeq 1$ cm). Also, in Ref. 24 it was pointed out that the limits on $q - 1 = \alpha$ were given as $\alpha < 2 \times 10^{-5}$ which was based on the primordial helium abundance and is of the same order of magnitude as that predicted by the CMB anisotropy.

3. *Conclusion*

The above discussion has given us an approach to the problem of how to deal with anharmonic perturbations for lattice vibrations in a solid at low T when the non-extensive statistics applies. The very low temperature domain leads to a simplifying condition since we only have to deal with the ground state and the first excited state. Also, for the modifications of the Einstein theory for the heat capacity due to the non-extensive statistics, we have to multiply Eq. (2.12) by $3N$ and differentiate with respect to T. The result is

$$C_v = 3N\left[\frac{k(b+c)^2}{(kT)^2}{\rm e}^{-(b+c)/(kT)}\right] \tag{2.20}$$

$$+3N\alpha\left[\frac{-(b+c)^2}{kT^2} + 2\frac{(b+c)^3}{k^2T^3} - \frac{(b+c)^4}{k^3T^4}\right]\ {\rm e}^{-(b+c)/(kT)}\,.$$

In Eq. (2.20), we have the measurable corrections to the heat capacity at low T [32] for solids that admit an anharmonic term and also have a multi-fractral structure admitting to non-extensive statistics. One problem is that the usual Einstein theory better fits the experimental data at higher temperatures when the solid can be thought of as vibrating in one mode. However, if the anharmonic term is large enough, we can imagine that the non-linearity can cause a coupling between all the atoms and thus generate one dominant mode at low T. The experimental problem is to search for such a system, and study it's low temperature heat capacity where the anharmonic term essentially creates a multi-fractral structure making it necessary to apply Tsallis statistics. For normal solids, if very precise measurements can be made, the validity of Eq. (2.16) could be compared with experiments to gain some measure of the non-extensive parameter. Since very low temperatures are now attainable in the low temperature laboratories [33], it seems worthwhile to ask if any anomalies in C_v might be explained in terms of the formulas derived in the present study. Also, the high temperature domain can be studied by integrating over n which makes the evaluation of Eq. (2.7) possible. The result of these integrals leads to parabolic cylinder functions whose asymptotic behaviour has to be carefully analyzed in order to make contact with experiment.

The testing ground for such high-temperature effects would be in the thermal radiation where non-linear effects of the electromagnetic field generate the anharmonic term leading to modifications of the equation of state at high T and also give rise to modifications of the scale-factors evolution in cosmology during the early radiation era [34]. Although a very complicated mathematical analysis would be necessary in terms of parabolic cylinder functions, the high temperature domain would bring to focus the influence of non-extensive statistics on cosmological evolution.

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ANHARMONIČKI OSCILATOR I DOROCZY-TSALLISOVA STATISTIKA NA NISKOTEMPERATURNOJ GRANICI

Uvođenjem popravaka četvrtog reda u Hamiltonovu funkciju harmoničkog oscilatora, proučavamo njihov učinak na toplinsku energiju anharmoničkog oscilatora u okviru Doroczy-Tsallisove statistike na niskotemperaturnoj granici.