Low temperature specific heat of glasses: A non-extensive approach

Ashok Razdan
Nuclear Research Laboratory
Bhabha Atomic Research Centre
Trombay, Mumbai- 400085

Abstract:
Specific heat is calculated using Tsallis Statistics. It is observed that it is possible to explain some low temperature specific heat properties of glasses using non-extensive approach. A similarity between temperature dependence of non-extensive specific heat and fractal specific heat is also discussed.

Motivation:
Non-extensive statistics is being increasingly used to explain anomalous behaviour observed in the properties of various physical systems. Tsallis statistics has been used to study physical systems/phenomena which include turbulence in plasma [1], Cosmic ray background radiation [2], self gravitating systems [3], econo-physics [4], electron-positron annihilation [5], classical and quantum chaos [6], linear response theory [7], Levy type anomalous super diffusion [8], thermalization of electron-phonon systems [9], low dimensional dissipative systems [10] etc. It has been shown that non-extensive features get manifested in those systems which have long range forces, long memory effects or in those systems which evolve in (non Euclidean like space-time) fractal space time [11 and references therein]. Apart from other applications it has been suggested [11] that non-extensive statistics can be applied to complex systems like glassy materials and fractal/multi-fractal or unconventional structures also. Anomalous low temperature specific heat results in glasses have motivated us to use non-
extensive statistics. We will also compare specific heat using Tsallis statistics with specific heat of a fractal.

**Low temperature specific heat:**

Specific heat depends on density of states \( g(\omega) \)

\[
C_p = k_B^2 \int_0^\infty g(\frac{k_B T}{\hbar} x) \frac{x^2 e^x}{(e^x - 1)^2} dx
\]

where \( x = \frac{\hbar \omega}{k_B T} \). Above equation has been obtained using Boltzmann Gibbs statistical mechanics. Glasses at low temperature (below 2K) show quasi-linear behaviour i.e. approximate linear dependence on temperature \( T \). Again glassy systems do not follow \( T^3 \) dependence even above 2K as in some cases maximum in \( \frac{C_p}{T^3} \) is observed. Above properties are universal features of glassy systems [12,13]. Another interesting feature is \( C_p T^2 \) dependence on \( T^2 \) for crystals and glassy phase of the same systems [14].

**Theory:**

Non-extensive statistics is based on two postulates [11 and reference therein]. First is the definition of non-extensive entropy

\[
S_q = \frac{1 - P_i^q}{q - 1}
\]

where \( q \) is the non-extensive entropic index and \( P_i \) are the probabilities of the microscopic states with \( \sum P_i = 1 \).

The second postulate is the definition of energy \( U_q = \sum P_i^q E_i \), where \( E_i \) is the energy spectrum. As \( q \to 1 \), \( S_q = - \sum p_i ln P_i \), which is the Boltzmann Gibbs Shannon entropy.

To derive non-extensive form of specific heat we have to use non-extensive quantum distribution function of bosons. It is very difficult to derive exact analytical expression for non-extensive distribution function. However, there are many studies which provide the approximate form of non-extensive distribution functions [2,15]. In the present paper we use dilute gas approximation (DGA) for boson distribution function. For DGA case, the average occupation number is given as [15]

\[
< n_q > = \frac{1}{(1 + (q - 1)\beta(\epsilon_i - \mu)^{\frac{1}{1-q}} - 1)}
\]
Figure 1: Non-extensive specific heat for various values of q: q=1.5(a),1.6(b),1.7(c),1.8(d), 1.9(e),2.0(f),2.5(g),3.0(h),3.5(k)

When dealing with system in contact with the heat bath at the temperature $\beta$, we have

$$\langle n_q \rangle = \frac{\hbar \omega_i}{(1 + (q-1) \frac{\hbar \omega_i}{kT})^{\frac{1}{q-1}}} - 1$$  \hspace{1cm} (4)

Averaged over non-extensive distribution, expectation value of energy is

$$\langle E_q \rangle = \hbar \omega < n_q >$$  \hspace{1cm} (5)

and total vibrational energy is

$$U_q = \int \hbar \omega < n_q > g(\omega)$$  \hspace{1cm} (6)

from which specific heat can be obtained

$$C_p = \frac{\partial U_q}{\partial T}$$  \hspace{1cm} (7)

For the case of Debye approximation $g(\omega) \propto (\omega)^2$. Equation (7) represents specific heat using Tsallis statistics where $n_q$ is given by equation (4).

**Results and Discussion:**

We have numerically solved equation (7) using equations (4) and (6), for various values of q. It is very clear from figure 1 that quasi-linear behaviour or maxima in $\frac{C_p}{T^3}$ is not explained by including non-extensive statistics. Various curves in figure 1 have been obtained for fixed value of Debye temperature
Figure 2: Fig2a: Sp. heat data corresponding to \((B_2O_3)_{100-x}(Na_2O)_x\) for different % of \(Na_2O\) [16,17,18] Fig2b: Sp. heat data corresponding to glassy alcohols [14,19]. In y-axis \(\frac{c_p}{T}\) is plotted against \(T^2\) in x-axis

\((\theta_D=300\text{ K})\). The shape and nature of curves in figure 1 is decided by value of q. A linear display of specific heat versus \(T^2\) dependence is followed in glasses as depicted in figure 2a and figure 2b. In figure 2a we are plotting experimental data corresponding to \((B_2O_3)_{100-x}(Na_2O)_x\) taken from reference [16,17,18]. The data with (+) sign corresponds to 0 % of \(Na_2O\), (*) corresponds to 1 % of \(Na_2O\), hollow square corresponds to 6 %, filled square corresponds to 16 % and crosses (x) corresponds to 25 % of \(Na_2O\) respectively. The fitted curves correspond to different values of q from (+)onwards are q=5.5, 5.0, 4.5, 3.5,3.0,2.9, 2.7,2.6 respectively. The slope of experimental data in figure 2a is strongly dependent on presence, absence or excess of \(Na_2O\) in glassy system. Non-extensive specific heat seems to explain data in figure 2a for different values of q. Again in figure 2b specific heat data of various glassy systems show strong dependence on slope and can be explained by non-extensive approach. The experimental data in fig2b corresponds to glassy alcohols like 2-proponal (+), filled square to D-ethonal, cross (x) to D-ethonal (OG, orientational glass), hollow square to 1-proponal and star (*) to glycerol respectively. The corresponding fitted q-values are q=2.8,2.65,2.62,2.60 and 2.25 respectively. The experimental data has been taken from reference [19,22]. It is interesting to mention here that a
In y-axis $\frac{\partial^2 \langle E \rangle}{\partial T^2}$ is plotted against $T^2$ in x-axis.
ported that quasi-linear behaviour or maximum in specific heat data of various incommensurate phases can be explained [25] by considering effect of phason damping.

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