Int J Theor Phys (2008) 47: 1954–1965
DOI 10.1007/s10773-007-9639-0

The Effect of Space Dimensions on a Generalized Hydrogen-Atom Specific Heat in the Generalized Boltzmann-Gibbs Statistics

M. Barati · N. Moradi

Received: 15 October 2007 / Accepted: 19 December 2007 / Published online: 3 January 2008

Abstract In this article, the effect of the space dimensions on the generalized hydrogen-atom specific heat in the generalized Boltzmann-Gibbs statistics is studied. The temperature dependence of the specific heat for a few different values of q and for different low space dimensions using Tsallis statistics is numerically calculated. The results indicate that for a fixed value of q, as the space dimension increases the temperature range where the specific heat has a nonzero value, decreases, while the general behavior of the specific heat does not show any change. Also, there exits a q-independent quantity related to two specific temperatures of the system which is almost linearly dependent on the space dimensions.

Keywords Specific heat · Generalized hydrogen-atom · Generalized Tsallis statistics · Dimensions of space

1 Introduction

It is known that there exist a variety of physical systems that Boltzmann-Gibbs (BG) statistical mechanics and standard thermodynamics [1] cannot explain [2, 3]. The list of such anomalies increases every day [4]. One set of the most important of such systems are those involving long-range interactions [5]. The generalized statistical mechanics and thermodynamics theories address this type of difficulty. The formalism proposed by C. Tsallis where the generalized entropy is expressed as [6]:

$$S_q = k\frac{1-\sum p_n^q}{q-1} \quad (q \in \mathbb{R},\ k \text{ is a positive constant}), \tag{1}$$

here $\{p_n\}$ are the probabilities of the microscopic configurations (if our system is a generic quantum one, $\{p_n\}$ are the eigenvalues of the density operator ρ). It should be mentioned that the entropy and therefore the other thermodynamic parameters approach the BG statistical

---

M. Barati (✉) · N. Moradi
Department of Physics, College of Science, Shiraz University, Shiraz 71454, Iran
e-mail: barati@susc.ac.ir

mechanics results in the $q \to 1$ limit [3, 7]. One of the distinct properties of the Tsallis entropy is that the entropy is non-additive. One can easily show that:

$$S_q(A+B)/k = [S_q(A)/k] + [S_q(B)/k] + (1-q)[S_q(A)/k][S_q(B)/k], \tag{2}$$

where A and B representing two independent systems (i.e., $\mathcal{H}(A+B) = \mathcal{H}(A) + \mathcal{H}(B)$, $\mathcal{H}$ is Hamiltonian, and $p_{ij}(A+B) = p_i(A)p_j(B)$). In this specific sense the parameter q characterizes the degree of the non-extensivity of the system, such that for $q = 1$ the entropy becomes extensive and approaches the standard form of the BG as expected. For a specific given correlation between A and B, a special value of $q = q^*$ might exit for which $S_{q^*}(A, B) = S_{q^*}(A) + S_{q^*}(B)$. Other interesting properties of Tsallis entropy has been discussed in detail by Gell-Mann and Tsallis et al. in [2]. In this article, systems consisting of elements with long-range interaction in different dimensions will be investigated. In D-space dimensions, for the systems including the two-body interactions in form of $\frac{1}{r^\alpha}$ ($\alpha > 0$), if $D < \alpha$ the interaction is short range and when $D > \alpha$ it is long range. The BG statistical mechanics can not explain many systems including long range interactions (weak violation of BG statistics). This is a situation that Tsallis formalism can be used [3].

2 The Hydrogen Atom in D-space Dimensions

The generalized Coulomb potential in D-space dimensions is proportional to $(-\frac{1}{r})$;

$$V(r) \propto -\frac{1}{r},$$

where

$$r^2 = \sum_{i=1}^{D} {x_i}^2. \tag{3}$$

With an appropriate choice of the system of units the Hamiltonian of a generalized hydrogen-atom in D- space dimensions can be written as:

$$\widehat{H} = -\frac{1}{2}\nabla^2 - \frac{1}{r}, \tag{4}$$

where

$$\nabla^2 = \sum_{i=1}^{D} {\nabla_i}^2. \tag{5}$$

The energy levels ($\varepsilon_{(n,D)}$) and degeneracy ($g_{(n,D)}$) of the states of the system are given in [8–10]:

$$\varepsilon_{(n,D)} = -\frac{R}{(n+\frac{D-3}{2})^2} \quad (n = 1, 2, 3, \ldots), \tag{6}$$

$$g_{(n,D)} = \frac{n(2n+D-3)(n+D-3)!}{n!(D-1)(D-2)!}, \tag{7}$$

where R is the Rydberg constant and $D \geq 2$. For $D = 3$ the familiar results ($\varepsilon_{(n,3)} = -\frac{1}{n^2}$ and $g_{(n,3)} = n^2$), are obtained as expected. As it was mentioned in Sect. 2, for $D = 2, 3, 4, 5, \ldots$

the Coulomb potential is a long-range interaction in all dimensions, because $\alpha = 1$ for the Coulomb potential and therefore $D > \alpha$. In the BG formalism it is easy to show that for this especial case (generalized hydrogen-atom) the partition function diverges [11], and therefore the BG statistics is not able to explain the thermodynamic properties of such a system but it is expected that generalized BG statistics be able to do this work.

3 Canonical Ensemble in Tsallis Statistics

Here a system in contact with a heat reservoir at temperature $T \equiv \frac{1}{\beta k}$ is considered. In order to obtain the thermal equilibrium probability distribution function in the Tsallis formalism, the Tsallis entropy must be optimized under appropriate constraints. The constraints are:

$$\sum_{n=1}^{W} p_n = 1 \quad \text{(normalization constraint)}, \tag{8}$$

$$\sum_{n=1}^{W} {p_n}^q \varepsilon_n = U_q \quad \text{(energy constraint)}, \tag{9}$$

where $\{\varepsilon_n\}$ are the eigenvalues of the Hamiltonian ($\mathcal{H}$), W is the total number of microscopic states and U_q is the generalized internal energy of the system (with this choice of U_q, in fact, we choose an un-normalized q-expectation values presentation). After optimization, the canonical distribution is obtained [12, 13] as:

$$p_{(\varepsilon_n)} = \begin{cases} \frac{g_n[1-\beta(1-q)\varepsilon_n]^{\frac{1}{1-q}}}{Z_q} & \text{if } [1-\beta(1-q)\varepsilon_n] > 0, \\ 0 & \text{otherwise,} \end{cases} \tag{10}$$

where $\{g_n\}$ are the degeneracies of the system associated with $\{\varepsilon_n\}$ and $\{Z_q\}$ is the generalized partition function and is given by:

$$Z_q \equiv \sum_{levels} g_i[1-\beta(1-q)\varepsilon_i]^{\frac{1}{1-q}}. \tag{11}$$

Equation (10) is not invariant under change of the zero level for energy spectrum $\{\varepsilon_n\}$, however we have chosen the ground state of energy at the origin similar to others. The expression of the equilibrium distribution is complemented by the auxiliary condition that $p_{\varepsilon_n} = 0$ whenever the argument becomes negative (cut-off condition), which occurs only for $q < 1$ [13]. This requirement (cut-off condition) plays a substantial role in our calculations. For the U_q defined by (9) the usual thermodynamics Legendre structure remains valid for all values of q [12]. So the generalized specific heat ($C_q = \frac{\partial U_q}{\partial T}$) is obtained as:

$$\frac{C_q}{k} = \frac{qZ^{1-q}(\langle E_n^2\rangle' - (\langle E_n\rangle')^2)}{(kT)^2} \tag{12}$$

with

$$E_n \equiv \frac{\varepsilon_n}{[1-\beta(1-q)\varepsilon_n]}, \tag{13}$$

where $\langle f(\varepsilon_n)\rangle'$ is defined as $\sum_{levels} p_{(\varepsilon_n)} f(\varepsilon_n)$. Furthermore, C_q has the sign of q ($\frac{C_q}{q} \geq 0$). You can find a similar BG relation of (12) in [1].

4 Discussion and Results

Here, the method presented in the previous section is applied to obtain the generalized hydrogen-atom specific heat in different space dimensions. This method has been applied for a real hydrogen atom ($D = 3$) by Lucena, da Silva and Tsallis [11]. We also consider the effect of the addition of the space dimensions on the generalized specific heat in some points.

As it has been mentioned in [11], today it seems to be impossible to predict the exact value of q for a non-ionized real hydrogen-atom in free space, since there is no experimental report on any of its thermodynamic parameters. However, for such self-gravitating system ($D = 3$), the upper range of q is mathematically well determined. This critical value is $\frac{7}{9}$ [11]. Since we are mostly interested in observing the dimensional effects on the generalized specific heat we will perform our calculations for three different typical values of q i.e. $q = 0.35$, $q = 0.5$, and $q = 0.65$. The energy states for the generalized hydrogen-atom with zero ground state energy is given as:

$$\varepsilon_{(n,D)} = R\left(\frac{1}{(\frac{D-1}{2})^2} - \frac{1}{(n+\frac{(D-3)}{2})^2}\right). \tag{14}$$

By substituting the above equation in (10) we obtain:

$$p_{(\varepsilon_n,D)} = \begin{cases} \dfrac{\frac{n(2n+D-3)(n+D-3)!}{n!(D-1)(D-2)!}[1-\frac{(1-q)}{t}(\frac{1}{(\frac{D-1}{2})^2}-\frac{1}{(n+\frac{(D-3)}{2})^2})]^{\frac{1}{1-q}}}{Z_q} \\ \quad \text{if } t > (1-q)\big(\frac{1}{(\frac{D-1}{2})^2} - \frac{1}{(n+\frac{(D-3)}{2})^2}\big), \\ 0 \quad \text{otherwise}, \end{cases} \tag{15}$$

where

$$t \equiv \frac{kT}{R} \tag{16}$$

and

$$Z_{(q,D)} = \sum_{levels} \frac{n(2n+D-3)(n+D-3)!}{n!(D-1)(D-2)!}\left[1-\frac{(1-q)}{t}\left(\frac{1}{(\frac{D-1}{2})^2} - \frac{1}{(n+\frac{(D-3)}{2})^2}\right)\right]^{\frac{1}{1-q}}. \tag{17}$$

The generalized specific heat is calculated from (12) as:

$$\frac{C_{(q,D)}}{k} = \frac{qz_q^{1-q}}{t^2}\left(\sum_{levels} p_{(\varepsilon_n,D)}\left(\frac{(\frac{1}{(\frac{D-1}{2})^2} - \frac{1}{(n+\frac{(D-3)}{2})^2})}{[1-\frac{(1-q)}{t}(\frac{1}{(\frac{D-1}{2})^2} - \frac{1}{(n+\frac{(D-3)}{2})^2})]}\right)^2\right)$$
$$- \frac{qz_q^{1-q}}{t^2}\left(\sum_{levels} p_{(\varepsilon_n,D)}\frac{(\frac{1}{(\frac{D-1}{2})^2} - \frac{1}{(n+\frac{(D-3)}{2})^2})}{[1-\frac{(1-q)}{t}(\frac{1}{(\frac{D-1}{2})^2} - \frac{1}{(n+\frac{(D-3)}{2})^2})]}\right)^2. \tag{18}$$

The anomalous behavior of the specific heat are seen at all dimensionless temperatures (see (16)) $t_{(n,D)} = (1-q)(\frac{1}{(\frac{D-1}{2})^2} - \frac{1}{(n+\frac{(D-3)}{2})^2})$ for $n = 2, 3, 4, \ldots$ and the different dimensions as can be seen in Figs. 1–8. In order to study the effect of the space dimensions on

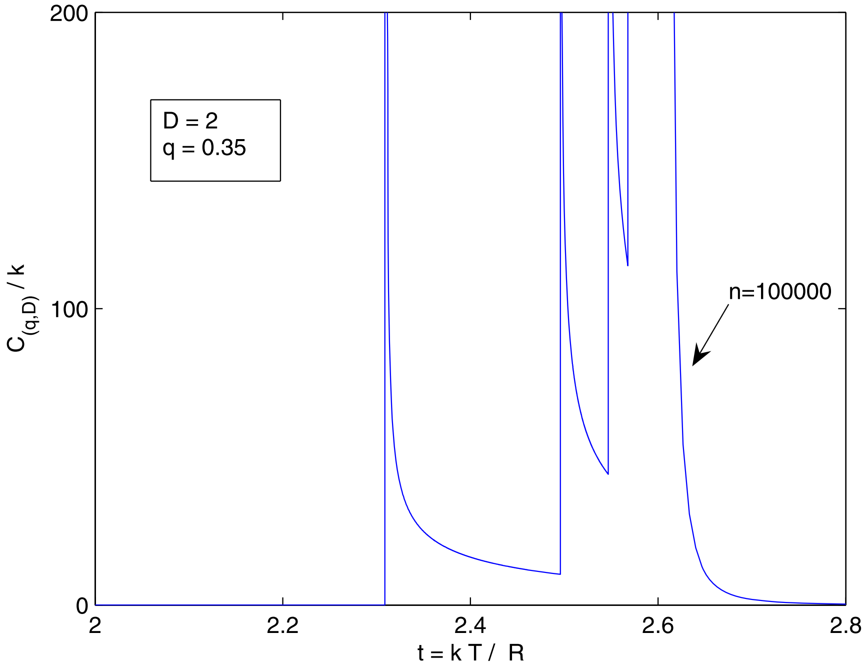

Fig. 1 $C_{(q,D)}/k$ versus t for $D=2$, $q=0.35$

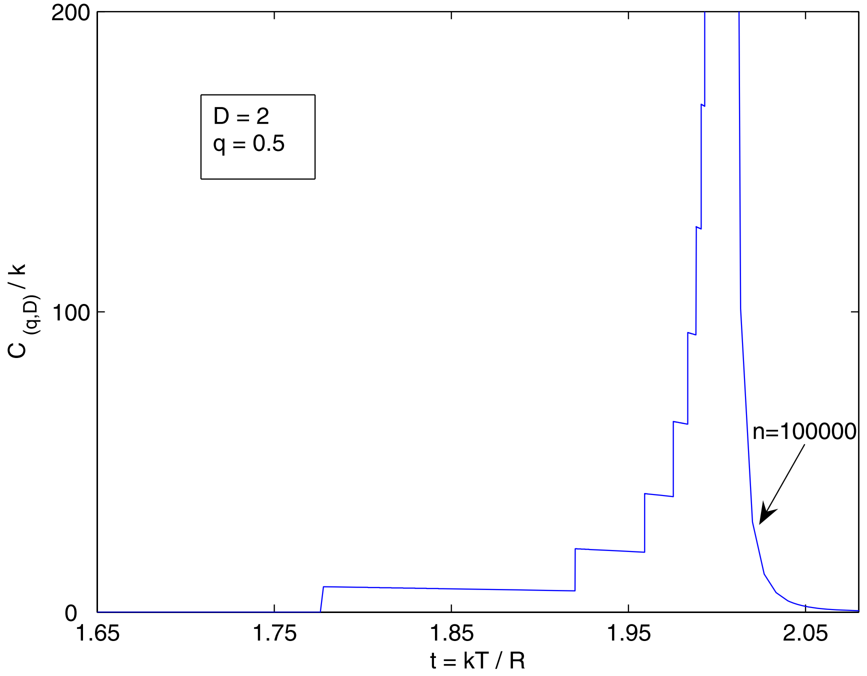

Fig. 2 $C_{(q,D)}/k$ versus t for $D=2$, $q=0.5$

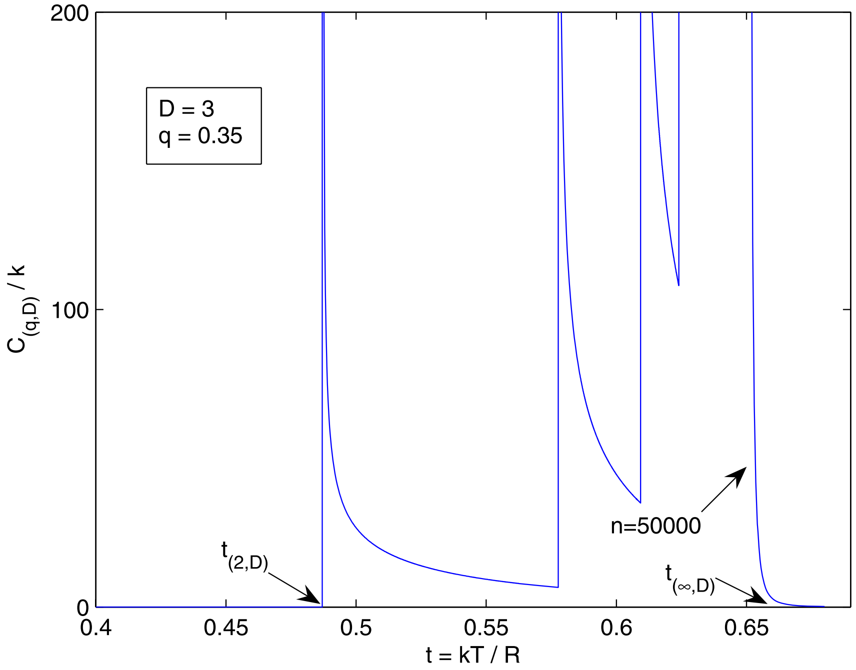

Fig. 3 $C_{(q,D)}/k$ versus t for $D = 3$, $q = 0.35$

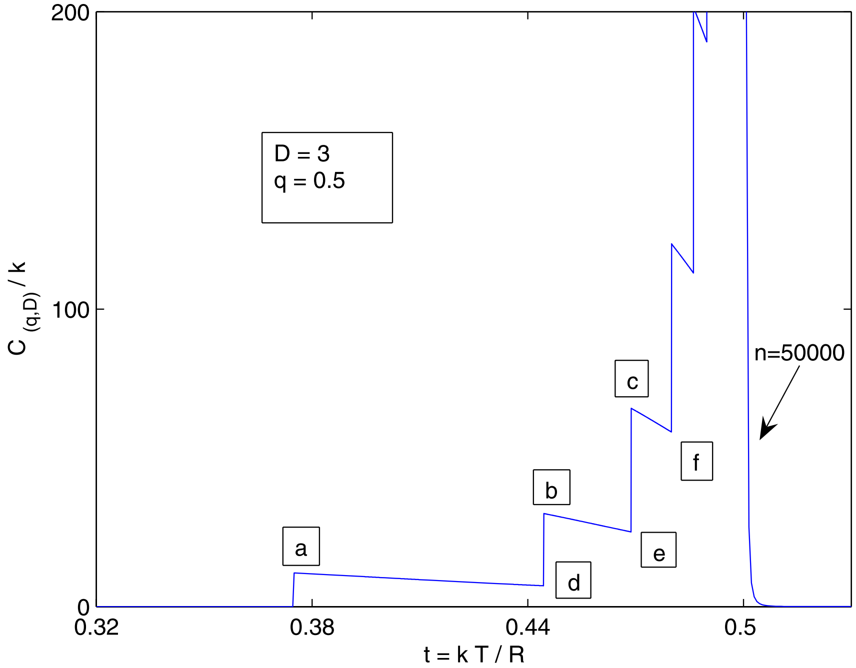

Fig. 4 $C_{(q,D)}/k$ versus t for $D = 3$, $q = 0.5$; a, b and c are local maxima; d, e and f are local minima

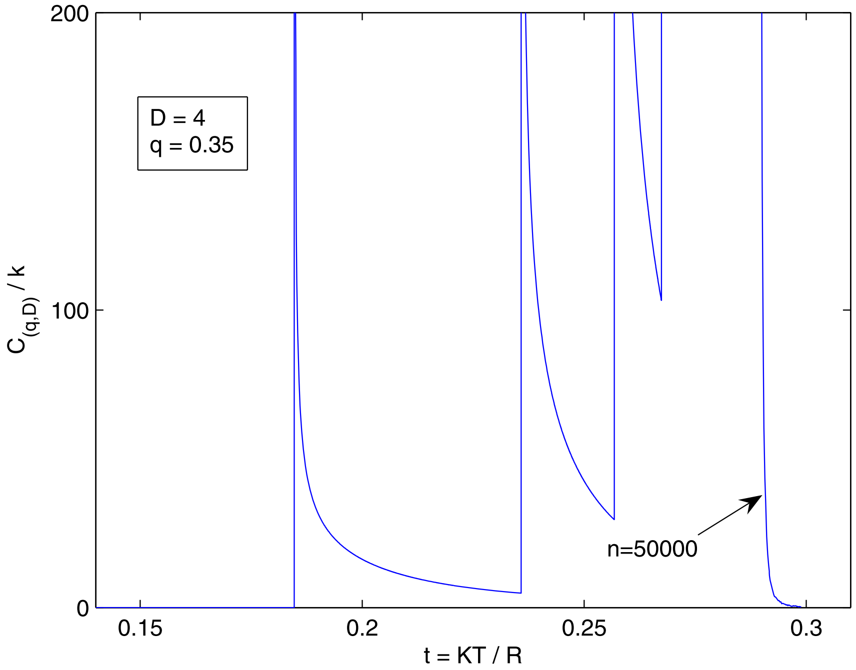

Fig. 5 $C_{(q,D)}/k$ versus t for $D = 4$, $q = 0.35$

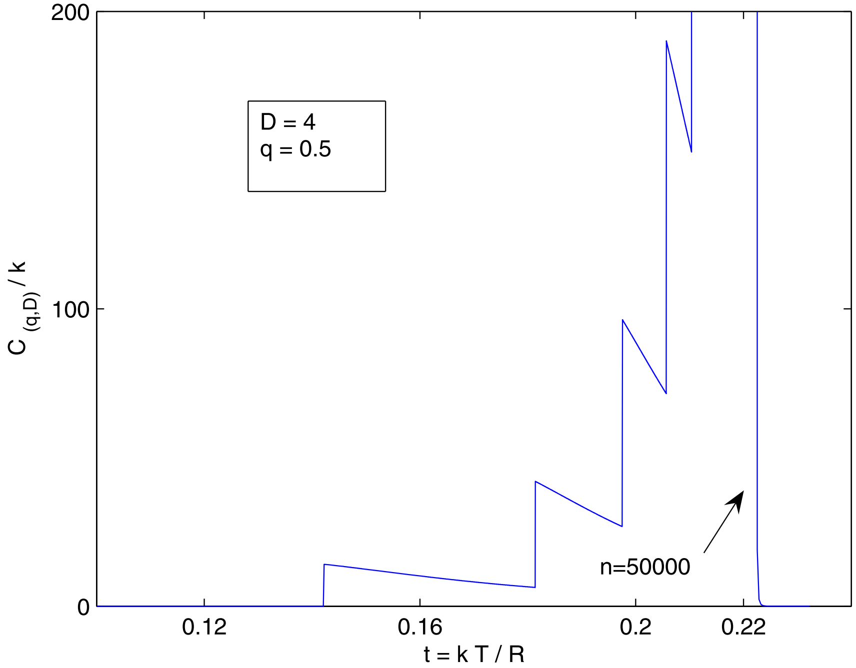

Fig. 6 $C_{(q,D)}/k$ versus t for $D = 4$, $q = 0.5$

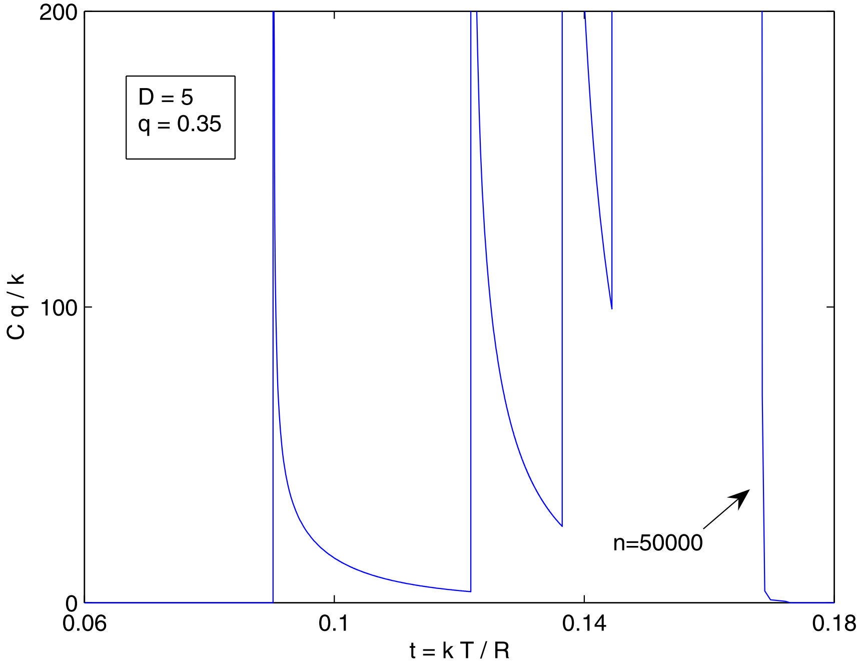

Fig. 7 $C_{(q,D)}/k$ versus t for $D = 5$, $q = 0.35$

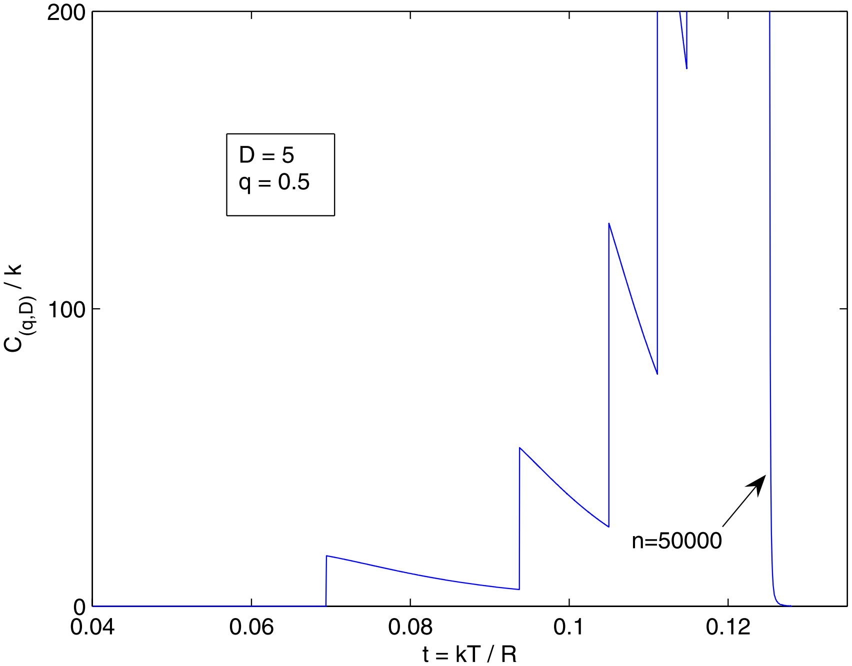

Fig. 8 $C_{(q,D)}/k$ versus t for $D = 5$, $q = 0.5$

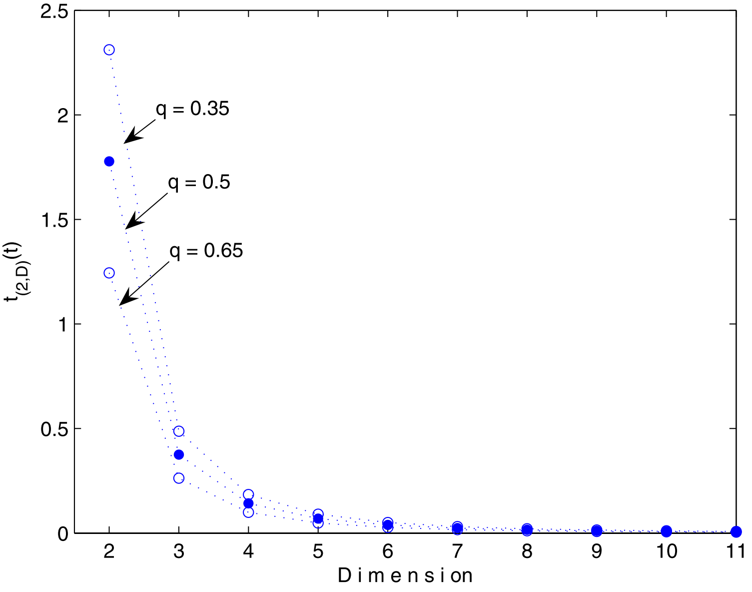

Fig. 9 $t_{(2,D)}$ versus D for $q = 0.35, 0.5, 0.65$

the specific heat, the behavior of the systems for two specific values of t, i.e. $t_{(2,D)}$ and $t_{(\infty,D)}$ is investigated. The first, $t_{(2,D)}$, is the lowest dimensionless temperature where $C_{(q,D)}$ is nonzero. This point can be identified from the above equation for $n = 2$. So $t_{(2,D)}$ is given as:

$$t_{(2,D)} = (1-q)\left(\frac{1}{(\frac{D-1}{2})^2} - \frac{1}{(\frac{D+1}{2})^2}\right) = (1-q)\frac{16D}{(D^2-1)^2}. \tag{19}$$

This result directly depends on the cut-off condition for $\sum$ in (15). The second dimensionless temperature is $t_{(\infty,D)}$, such that for $t > t_\infty$ the number of the terms in $\sum$ diverges without any cut-off in (18). In fact, the maximum value of $C_{(q,D)}$ occurs at this point and it vanishes for $t > t_\infty$ as can be seen in Figs. 1–8. The value of $t_{(\infty,D)}$ can be determined by the previous equation for $t_{(n,D)}$ in the $n \to \infty$ limit, so:

$$t_{(\infty,D)} = (1-q)\left(\frac{1}{(\frac{D-1}{2})^2}\right), \tag{20}$$

$t_{(2,D)}$ versus the space dimension (D) for $q = 0.35$, $q = 0.5$, and $q = 0.65$ has been shown in Fig. 9. As it can be seen from the figure, $t_{(2,D)}$ strongly depends on the value of q for small dimensions. For large dimensions, $t_{(2,D)}$ approaches zero as $\frac{1}{D^3}$ and is independent of q. The behavior of $t_{(\infty,D)}$ as a function of D has been shown in Fig. 10. The behavior is almost the same as for $t_{(2,D)}$, but in this case, $t_{(\infty,D)}$ approaches zero as $\frac{1}{D^2}$. The effect of the space dimension (D) on the first, second and the third local maxima of the $C_{(q,\infty)}$ and the same effect for the local minima for $q = 0.5$ have been shown in Fig. 11 and Fig. 12 respectively. As it can be seen from the figures the local maxima monotonically increase as the space dimension increases, but the local minima indicate a non monotonic behavior with slower variation rate than the local maxima.

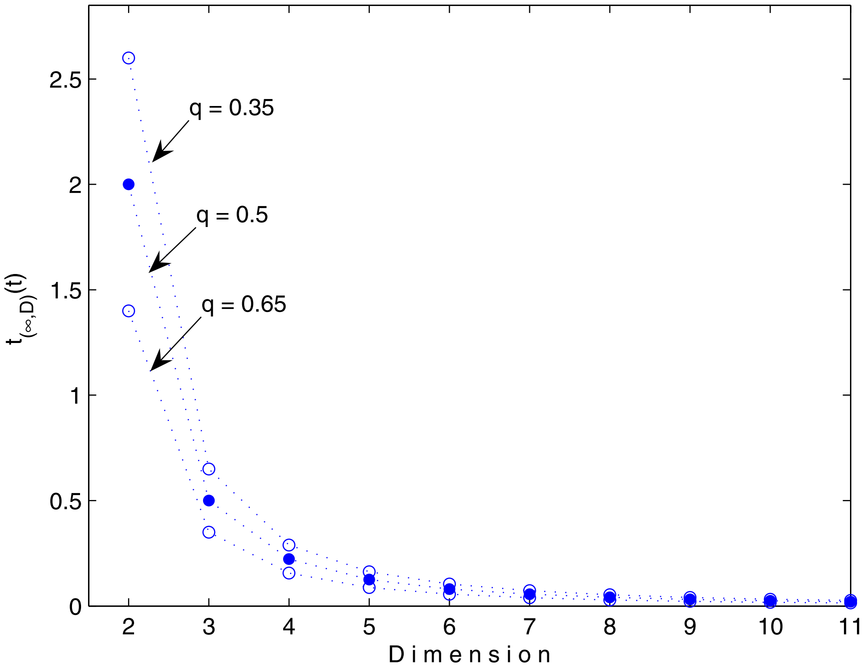

Fig. 10 $t_{(\infty,D)}$ versus D for $q = 0.35, 0.5, 0.65$

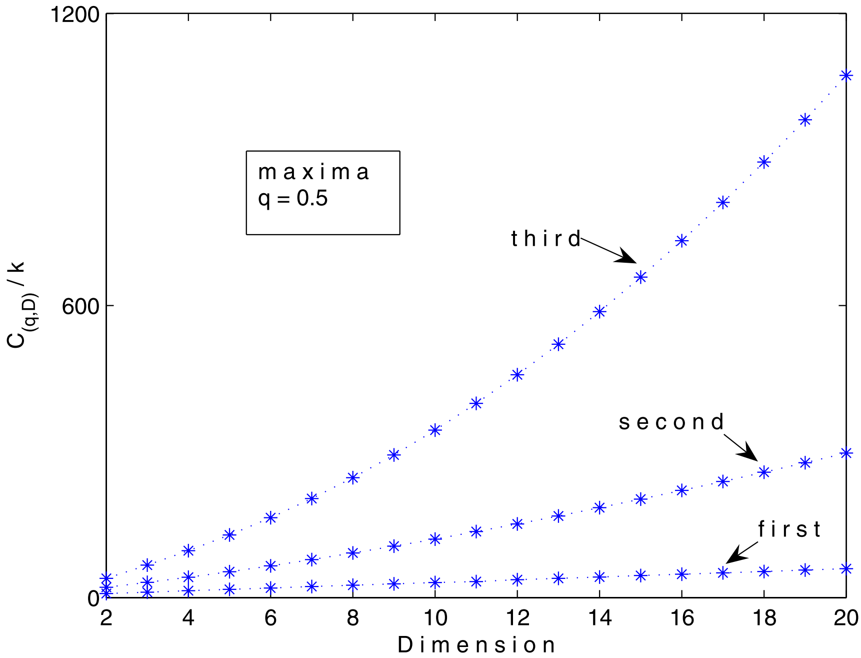

Fig. 11 The values of local maxima versus D for $q = 0.5$

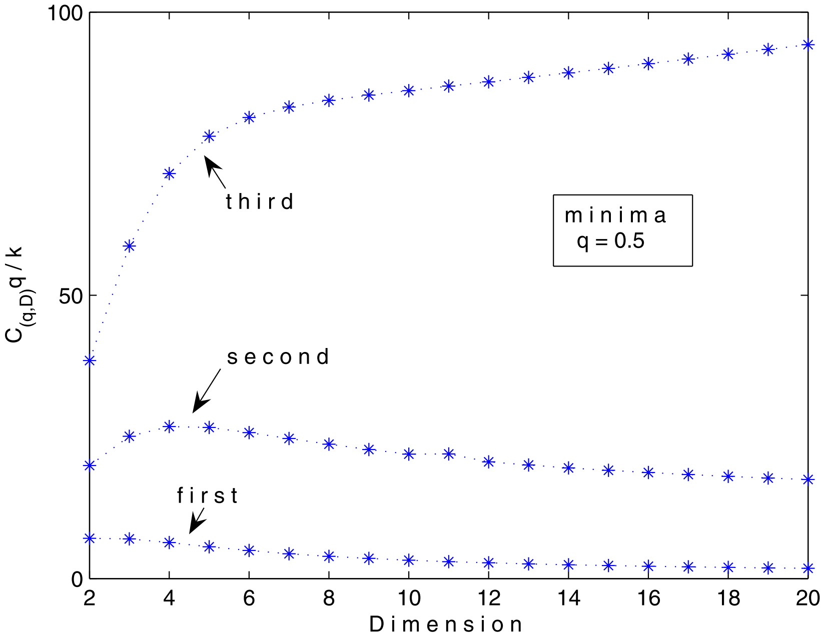

Fig. 12 The values of local minima versus D for $q = 0.5$

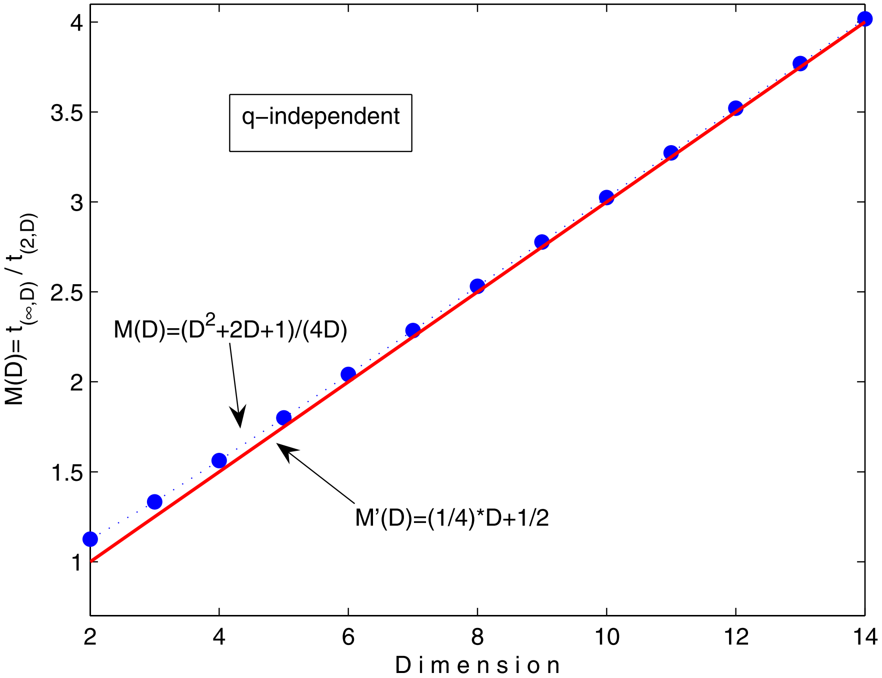

Fig. 13 $M(D) = \frac{t_{(\infty,D)}}{t_{(2,D)}}$ versus D (independent of q)

At the end the ratio

$$M(D) \cong \frac{t_{(\infty,D)}}{t_{(2,D)}} = \frac{D^2+2D+1}{4D}, \tag{21}$$

as a function of the space dimension (D) is investigated. This ratio is independent of q and linearly increases for large dimensions as it can be seen from Fig. 13.

5 Conclusion

The effect of the space dimensions on the generalized hydrogen-atom specific heat in the generalized Boltzmann-Gibbs statistics was studied. The results indicate that as the dimension of the space (D) increases, the range of temperature with nonzero values of the specific heat decreases as $\frac{1}{D^2}$ and the value of the local maxima increases monotonically as the dimension increases. It is also interesting to mention that the ratio of $t_{(\infty,D)}$ corresponding to the highest temperature, to $t_{(2,D)}$ corresponding to the lowest temperature with nonzero specific heat is independent of q and depends almost linearly on the space dimension.

References

1. Pathria, R.K.: Statistical Mechanics, 2nd edn. Butterworth-Heinemann, Oxford (1996)
2. Gell-Mann, M., Tsallis, C.: Nonextensive Entropy-Interdisciplinary Application. Oxford University Press, New York (2004)
3. Abe, S., Okamoto, Y.: Nonextensive Statistical Mechanics and Its Application. Springer, Berlin (2001)
4. An up-to-date reference list for new researches in Tsallis statistics is available at http://tsallis.cat.cbpf.br (2007)
5. Saslaw, W.C.: Gravitational Physics of Stellar and Galactic Systems. Cambridge University Press, Cambridge (1984)
6. Tsallis, C.: J. Stat. Phys. **52**, 479 (1988)
7. Curado, E.M.F., Tsallis, C.: J. Phys. A **24**, L69 (1991). Corrigenda: **24**, 3187 (1991) and **25**, 1019 (1992)
8. Al-Jaber, S.M.: Int. J. Theor. Phys. **37**, 1289 (1998)
9. Nieto, M.M.: Am. J. Phys. **47**, 1067 (1979)
10. Kibler, M.R.: quant-ph/0409209 (2004)
11. Lucena, L.S., da Silva, L.R., Tsallis, C.: Phys. Rev. E **51**, 6247 (1995)
12. da Silva, E.P., Tsallis, C., Curado, E.M.F.: Physica A **199**, 137 (1993)
13. Tsallis, C., Mendes, R.S., Plastino, A.R.: Physica A **261**, 534 (1998)