The role of curvature in quantum statistical mechanics

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Abstract. In this manuscript, we calculate the scalar curvature of a two-dimensional thermodynamic space to study the properties of two thermodynamic systems. In particular, we study the stability and possible anyonic behavior of quantum group invariant systems and systems with fractal distribution functions.

1. Introduction

During the last five decades there has been a lot of development in using geometry to study some properties of thermodynamic systems [1]-[5]. In particular, it consists in defining a metric in a two dimensional parameter space and calculate the corresponding scalar curvature as a measure of the correlations strength of the system [7]-[15], with applications to classical and quantum gases [6][12][16][17], magnetic systems [18]-[21], non-extensive statistical mechanics [22]-[24], anyon gas, fractional statistics and deformed boson and fermion systems [25], systems with fractal distribution functions [26], quantum group invariant systems [27], systems with M-statistics [28], and those related to Dunkl differential-difference operators [29]. Some of the basic results of these approaches include the relationships between the metric with the correlations of the stochastic variables, and the scalar curvature R with the stability of the system, and the facts that the scalar curvature R vanishes for the classical ideal gas, $R > 0 (R < 0)$ for a boson (fermion) ideal gas, and it is singular at a critical point. In Section 2 we give a general but brief introduction to the calculation of the thermodynamic metric and the corresponding scalar curvature. In Sections 3 and 4 we apply the formalism to study the stability and possible anyonic behavior for the cases of quantum group invariant systems and systems with fractal distribution functions, respectively. In constrast to the quantum group case the fractal density distribution is not exponential.


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2. Thermodynamic curvature

In order to make the discussion as general as possible, we start with a general probability density ρ which is not necessarily exponential. Therefore, let us define

$$\rho = \frac{1}{Z}\prod_{l=0} F_l. \tag{1}$$

Starting with the relative entropy for two close densities $\rho(\beta^\alpha)$ and $\rho(\beta_\alpha + d\beta_\alpha)$, where $\beta_1 = \beta$ and $\beta_2 = -\beta\mu$, (two-dimensional coordinate space). The metric is defined [7] as the second order term in the expansions of the information distance

$$I = Tr\rho\left(\ln\rho(\beta^\alpha) - \ln\rho(\beta^\alpha + d\beta^\alpha)\right). \tag{2}$$

Expanding, at second order we obtain the metric

$$g_{\alpha\gamma} = \frac{\partial^2 \ln Z}{\partial\beta_\alpha\partial\beta_\gamma} - Tr\left(\rho\sum_{l=0}\frac{\partial^2 \ln F_l}{\partial\beta_\alpha\partial\beta_\gamma}\right), \tag{3}$$

where the second term vanishes for exponential distributions with an exponent linear in the inverse temperature β. The scalar curvature R is given by

$$R = \frac{2}{detg}R_{1212}, \tag{4}$$

where the Riemann tensor reduces to

$$R_{\alpha\beta\gamma\delta} = g^{\eta\theta}(\Gamma_{\eta\gamma\lambda}\Gamma_{\theta\beta\gamma} - \Gamma_{\eta\alpha\gamma}\Gamma_{\theta\beta\lambda}) \tag{5}$$

The calculation of R simply reduces to solve the following determinant

$$R = \frac{1}{2(detg)^2}\begin{vmatrix} g_{11} & g_{22} & g_{12} \\ g_{11,1} & g_{22,1} & g_{21,1} \\ g_{11,2} & g_{22,2} & g_{21,2} \end{vmatrix}, \tag{6}$$

where $g_{\alpha\beta,\lambda} = \partial g_{\alpha\beta}/\partial\beta_\lambda$. The scalar curvature values give us the following information: Classical case: $R = 0$, Bosons: $R > 0$, Fermions :$R < 0$, at a phase transition: $R \to \infty$, and $R \approx 0$ implies a more stable system.

3. Geometry of Quantum Group invariant systems

In the last twenty years there has been considerable interest on applications of quantum groups [30][31], in addition to the theory of integrable models, to diverse areas of theoretical physics. The vast published literature on this subject includes formulations of quantum group versions of Lorentz and Poincaré algebras [32], its use as internal quantum symmetries in quantum mechanics and field theories [33], molecular and nuclear physics [34], and the formulation and study on the implications of imposing quantum group invariance in thermodynamic systems [35]. In particular, it has been shown [36] that quantum group gases exhibit anyonic behavior in two and three dimensions.

More recent applications include gravity theories wherein the discreteness and non-commutative properties of space-time at the Planck scale are approached mathematically by replacing the local symmetry by a quantum group symmetry [37] and applications to the phenomena of entanglement [38]. In particular,we focuses on the quantum group $SU_q(2)$ which consists of the set of matrices $T = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ with elements $\{a, b, c, d\}$ generating the algebra

$$ab = q^{-1}ba, \;\; ac = q^{-1}ca, \;\; bc = cb, \;\; dc = qcd, \;\; db = qbd,$$
$$da - ad = (q - q^{-1})bc, \;\; det_q T \equiv ad - q^{-1}bc = 1,$$

with the unitary conditions [39] $\overline{a} = d, \overline{b} = q^{-1}c$ and $q \in \mathbf{R}$. Hereafter, we take $0 < q < \infty$.

3.1. $SU_q(2)$-bosons

The $SU_q(2)$-invariant bosonic algebra is given by the following relations:

$$\Phi_2\overline{\Phi}_2 - q^2\overline{\Phi}_2\Phi_2 = 1, \;\; \Phi_1\overline{\Phi}_1 - q^2\overline{\Phi}_1\Phi_1 = 1 + (q^2 - 1)\overline{\Phi}_2\Phi_2,$$
$$\Phi_2\Phi_1 = q\Phi_1\Phi_2, \;\; \Phi_2\overline{\Phi}_1 = q\overline{\Phi}_1\Phi_2.$$

The simplest Hamiltonian written in terms of the operators Φ_j is simply written as

$$\mathcal{H}_B = \sum_\kappa \varepsilon_\kappa(\mathcal{N}_{1,\kappa} + \mathcal{N}_{2,\kappa}), \tag{7}$$

where $[\overline{\Phi}_{i,\kappa}, \Phi_{\kappa',j}] = 0$ for $\kappa \neq \kappa'$ and $\mathcal{N}_{i,\kappa} = \overline{\Phi}_{i,\kappa}\Phi_{i,\kappa}$. For a given κ the $SU_q(2)$ bosons are written in terms of boson operators ϕ_i and $\phi_i^\dagger$ with usual commutation relations: $[\phi_i, \phi_j^\dagger] = \delta_{ij}$ as follows

$$\Phi_j = (\phi_j^\dagger)^{-1}\{N_j\}q^{N_{j+1}}, \quad \overline{\Phi}_j = \phi_j^\dagger q^{N_{j+1}}, \quad j = 1, 2$$

leading to the interacting boson Hamiltonian

$$\mathcal{H}_B = \sum_\kappa \frac{\varepsilon_\kappa}{q^2 - 1} \sum_{m=1}^{\infty} \frac{2^m \ln^m q}{m!} \left(N_{1,\kappa} + N_{2,\kappa}\right)^m, \tag{8}$$

where $N_{i,\kappa}$ is the ordinary boson number operator and the q-number $\{n\} = \frac{1-q^{2n}}{1-q}$. Equation (7) becomes the standard free boson hamiltonian at $q = 1$.

The grand partition function $\mathcal{Z}_B$ is given by

$$\begin{aligned} \mathcal{Z}_B &= Tr\; e^{-\beta\sum_\kappa \varepsilon_\kappa(\mathcal{N}_{1,\kappa}+\mathcal{N}_{2,\kappa})} \\ &= \prod_\kappa \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} e^{-\beta\varepsilon_\kappa\{n+m\}} e^{\beta\mu(n+m)}, \end{aligned} \tag{9}$$

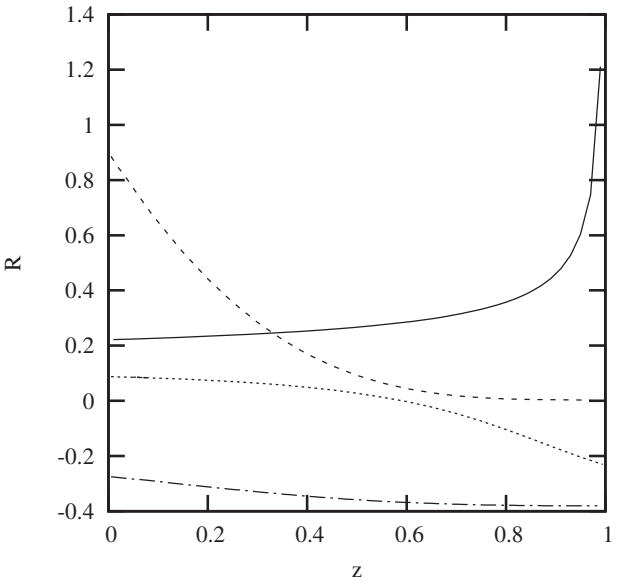


Figure 1. The scalar curvature R, in units of $\lambda^3 V^{-1}$, as a function of the fugacity z for quantum group bosons at $D = 3$ and constant β for the cases of $q = 1$ (solid line), $q = 0.5$ (dashed line) and $q = 1.15$ (dotted line) and $q = 2$ (dashed-dotted line).

which after rearrangement simplifies to the Equation

$$\mathcal{Z}_B = \prod_{\kappa} \sum_{m=0}^{\infty} (m+1) e^{-\beta \varepsilon_\kappa \{m\}} z^m, \tag{10}$$

where $z = e^{\beta\mu}$ is the fugacity. Since the density distribution is exponential, the second term in Equation (3) vanishes. The scalar curvature for $D = 2, 3$ is given by the Equation

$$R_D = \frac{(D+4\nu)\pi^\nu \lambda^D}{V_D} \left(\frac{c_\nu b_\nu^2 + a_\nu d_\nu b_\nu - 2 a_\nu c_\nu^2}{[(D+4\nu) a_\nu c_\nu - (D+2\nu-1) b_\nu^2]^2} \right), \tag{11}$$

where $\nu = \frac{D-2}{2}$ and for example

$$a_\nu = \int_0^\infty x^\nu \ln \left(1 + \sum_{n=1} (n+1) e^{-x\{n\}} z^n \right) dx, \tag{12}$$

where b_ν, c_ν and d_μ are obtained by taking the corresponding derivatives with respect to β_1 and β_2. Figures 1 displays the results of a numerical calculation of Equation (11) for the scalar curvature of a QGB system in $D = 3$. Figure 1 shows that for $0 < q \leq 1$ the curvature is positive for all z values, and therefore the system is bosonic. In addition, the system becomes more stable than the standard Bose-Einstein case at higher values of z. For $1 < q \approx 1.2$ the system exhibits anyonic behavior as a function of z and becomes purely fermionic for all values of z and $q > 1.2$. The calculation of the Equation (11) for $D = 2$ shows that for $0 < q < 1$ the system is bosonic and more stable at $z \approx 1$ than the standard case $q = 1$. For $q > 1$ the system goes from bosonic to fermionic and becomes bosonic becoming more unstable as z approaches the value of 1.

3.2. $SU_q(2)$-fermions
The $SU_q(2)$ invariant fermionic algebra is defined by the set of relations

$$\{\Psi_2, \overline{\Psi}_2\} = 1, \quad \{\Psi_1, \overline{\Psi}_1\} = 1 - (1 - q^{-2})\overline{\Psi}_2\Psi_2$$
$$\Psi_1\Psi_2 = -q\Psi_2\Psi_1, \quad \overline{\Psi}_1\Psi_2 = -q\Psi_2\overline{\Psi}_1$$
$$\{\Psi_1, \Psi_1\} = 0 = \{\Psi_2, \Psi_2\}.$$

The corresponding Hamiltonian in terms of the operators Ψ_i is simply

$$\mathcal{H}_F = \sum_\kappa \varepsilon_\kappa(\mathcal{M}_{1,\kappa} + \mathcal{M}_{2,\kappa}), \tag{13}$$

where $\mathcal{M}_{i\kappa} = \overline{\Psi}_{i,\kappa}\Psi_{i,\kappa}$ and $\{\overline{\Psi}_{\kappa,i}, \Psi_{\kappa',j}\} = 0$ for $\kappa \neq \kappa'$. The occupation numbers are restricted to $m = 0, 1$ and therefore $SU_q(N)$ fermions satisfy the Pauli exclusion principle. A simple check shows that the $SU_q(2)$ fermionic algebra is consistent with the following representation of Ψ_i operators in terms of fermion operators ψ_j

$$\Psi_2 = \psi_2, \quad \overline{\Psi}_2 = \psi_2^\dagger$$
$$\Psi_1 = \psi_1\left(1 + (q^{-1} - 1)M_2\right), \quad \overline{\Psi}_1 = \psi_1^\dagger\left(1 + (q^{-1} - 1)M_2\right)$$

where $M_2 = \psi_2^\dagger\psi_2$.

From Equation (13) we see that the original Hamiltonian becomes the interacting Hamiltonian

$$H_F = \sum_\kappa \varepsilon_\kappa\left(M_{1,\kappa} + M_{2,\kappa} + (q^{-2} - 1)M_{1,\kappa}M_{2,\kappa}\right). \tag{14}$$

Therefore the parameter $q \neq 1$ mixes the two degrees of freedom in a nontrivial way through a quartic term in the Hamiltonian.

The grand partition function $\mathcal{Z}_F$ is written

$$\begin{aligned}\mathcal{Z}_F &= \prod_\kappa \sum_{n=0}^{1}\sum_{m=0}^{1} e^{-\beta\varepsilon_\kappa(n+m-(1-q^{-2})mn}e^{\beta\mu(n+m)} \\ &= \prod_\kappa\left(1 + 2e^{-\beta(\varepsilon_\kappa-\mu)} + e^{-\beta\left(\varepsilon_\kappa(q^{-2}+1)-2\mu\right)}\right)\end{aligned} \tag{15}$$

which for $q = 1$ becomes the square of a single fermion type grand partition function. Figure 2 is a graph of R vs. q for the values $z = 0.1, 0.5, 2, 10$. For $z = 0.1$ the system becomes bosonic for $q \geq 2.3$. This QGF system is more stable than the $q = 1$ system when $q < 1$ and it is more unstable than the $q = 1$ system when $q > 1$. On the other hand, quantum group, $SU_q(2)$, fermions do not exhibit anyonic behavior at $D = 2$. However, a calculation of the virial coefficients for the two parameter case reveals that $SU_{q/p}(2)$ fermions have anyonic behavior [40].

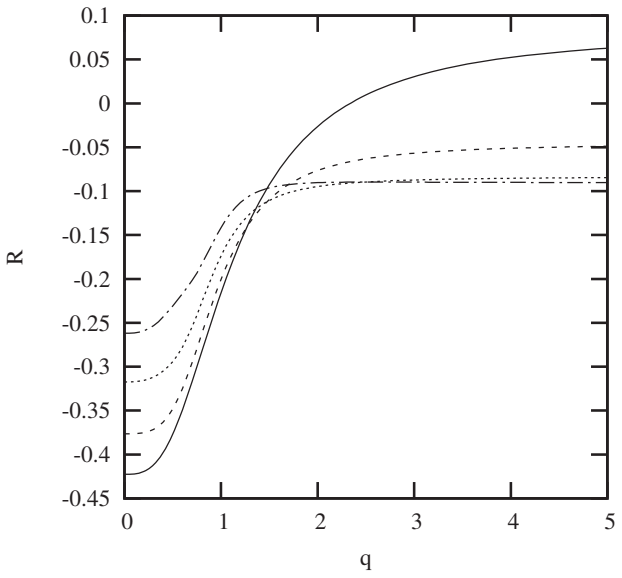


Figure 2. The scalar curvature R for quantum group fermions at $D = 3$, in units of $\lambda^3 V^{-1}$, as a function of the parameter q and values for the fugacity $z = 0.1$ (solid line), $z = 0.5$ (dashed line), $z = 2$ (dotted line) and $z = 10$ (dashed-dotted line).

4. Geometry of systems with fractal distribution functions

From the theory of fractals [41] we learned that given a statistical weight $\Omega(q, \delta)$ of a system with order parameter q and resolution δ, the fractal dimension is defined as the exponent $d = D_q$ which will make the product $lim_{\delta \to 0} \Omega(q, \delta)\delta^d$ finite. With use of the definition of the Boltzmann entropy $S(q, \delta) = \ln \Omega(q, \delta)$, the relation between the entropy and the fractal dimension D_q is given by

$$D_q = -\lim_{\delta \to 0} \frac{S(q, \delta)}{\ln \delta}. \tag{16}$$

Based on these definitions and with use of the Boltzmann's H theorem, the generalized entropy and distribution functions for classical and quantum gases were calculated in Ref.[42]. The average number of particles with energy ϵ was shown to be given by

$$< n(\epsilon) >= \frac{1}{\rho_j + a}, \tag{17}$$

where $\rho_j = [1 + \beta(q-1)(\epsilon - \mu)]^{1/(q-1)}$, $a = 0$ for the classical case, and the values $a = -1$ and $a = 1$ correspond to Bose-Einstein and Fermi-Dirac cases, respectively. For $q = 1$, Equation (17) becomes the standard textbook result for classical and quantum ideal gases. The distribution functions in Equation (17) were also obtained in Ref.[43] by considering a dilute gas approximation to the partition function of a non-extensive statistical mechanics originally proposed in Ref.[44]. In this Section we calculate the scalar curvature of systems with average particle number according to Equation (17). The probability densities that leads to Equation (17) were obtain in Ref. [45] and they are given by

$$\rho_{MB} = \frac{1}{Z_{MB}} \prod_{j=0} \frac{1}{n_j!} \rho^{-n_j}, \tag{18}$$

for the classical case, and

$$\hat{\rho} = \frac{1}{Z} \prod_{j=0} \rho^{-\hat{n}_j}, \tag{19}$$

for the Bose-Einstein and Fermi-Dirac cases. Since the density distribution is not exponential, the second term in Equation (3) does not vanish and the metric for the three cases can be summarized in the general formula [26]

$$g_{\alpha\gamma} = \sum_{l=0} \frac{< n_l >^2}{\rho_l} \frac{\partial \rho_l}{\partial \beta^\alpha} \frac{\partial \rho_l}{\partial \beta^\gamma}. \tag{20}$$

The curvature is given by the expression

$$R = \frac{\lambda^3}{4V(detg)^2} \left(5h_{1/2}h_{3/2}^2 - 6h_{1/2}^2 h_{5/2} + h_{3/2}h_{-1/2}h_{5/2} \right), \tag{21}$$

where the function

$$h_\lambda = \frac{2}{\sqrt{\pi}(q-1)^{(\lambda+1)}} \frac{\Gamma(\lambda+1)\Gamma(\frac{q}{q-1} - \lambda)}{\Gamma(\frac{2q-1}{q-1})} \frac{1}{[1+(q-1)\gamma]^{\frac{q}{q-1}-\lambda}}. \tag{22}$$

After replacement of the definition of the function h_λ we get that the scalar curvature for the classical fractal case is identically equal to zero. Therefore, in this case the parameter q does not play any role as far as correlations are concerned.

For the bosonic and fermionic cases the functions h_λ are replaced in Equation (21) by the functions

$$G_\lambda^\pm = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^\lambda \Omega^{\frac{3-2q}{q-1}}}{(\Omega^{\frac{1}{q-1}} \pm 1)^2} dx, \tag{23}$$

where the $(+)$ sign is for fermions and the $(-)$ sign for bosons, and the function $\Omega = 1 + (q-1)(x - \beta\mu)$. Numerical calculations for the boson and fermion systems show that the corresponding values of R as a function of the fugacity z are closer to zero than those in the $q = 1$ case, implying that the departure from the value $q = 1$ makes the systems more stable. Therefore, for $q \neq 1$ bosons will be less attractive and fermions less repulsive that their standard counterparts. Our results also show that the sign of R remains unchanged as a function of z implying that these systems do not exhibit anyonic behavior, a fact that looks impossible to check by performing an expansion for $z \approx 0$ to obtain the second virial coefficient because the partition function is a function of $\ln z$.

We can summarize that the two interesting systems are two examples of the usefulness of the calculation of the thermodynamic curvature. These calculations give us important information about the stability and possible anyonic behavior of the system under study as a function of the temperature and the particular additional parameter involved.

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