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ENTROPY MAXIMISATION PROBLEM FOR QUANTUM RELATIVISTIC PARTICLES

BY MIGUEL ESCOBEDO, STÉPHANE MISCHLER & MANUEL A. VALLE

ABSTRACT. — The entropy of an ideal gas, both in the case of classical and quantum particles, is maximised when the number particle density, linear momentum and energy are fixed. The dispersion law energy to momentum is chosen as linear or quadratic, corresponding to non-relativistic or relativistic behaviour.

RÉSUMÉ (*Maximisation d'entropie pour particules relativistes quantiques*)
L'entropie d'un gaz idéal de particules, classiques ou quantiques, est maximisée lorsque la densité du nombre de particules, l'impulsion et l'énergie sont fixées. La loi de dispersion qui relie l'impulsion et l'énergie est linéaire ou quadratique, selon que le comportement des particules est non relativiste ou relativiste.

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MIGUEL ESCOBEDO, Departamento de Matemáticas, Universidad del País Vasco, Apartado 644 Bilbao 48080 (Spain) • *E-mail :* mtpesmam@lg.ehu.es
STÉPHANE MISCHLER, Ceremade, Université Paris IX-Dauphine, place du Maréchal de Lattre de Tassigny, 75016 Paris(France) • *E-mail :* mischler@ceremade.dauphine.fr
MANUEL A. VALLE, Departamento de Física Teórica e Historia de la Ciencia, Universidad del País Vasco, Apartado 644 Bilbao 48080 (Spain) • *E-mail :* wtpvabam@lg.ehu.es

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1. Introduction

We are interested in the maximisation problem for the *quantum* or *non-quantum* entropy functional

$$H(g) := \int_{\mathbb{R}^3} h\big(g(p)\big)\,\mathrm{d}p, \quad h(g) = \tau^{-1}(1+\tau g)\ln(1+\tau g) - g\ln g, \tag{1.1}$$

where $\tau \in \mathbb{R}$, under the *relativistic* or *non-relativistic* moments constraint

$$\begin{pmatrix} N(g) \\ P(g) \\ E(g) \end{pmatrix} := \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ p \\ \mathcal{E}(p) \end{pmatrix} g(p)\,\mathrm{d}p = \begin{pmatrix} N \\ P \\ E \end{pmatrix}, \tag{1.2}$$

where $N > 0$ is the total number (or mass) of particles, $P \in \mathbb{R}^3$ is the mean momentum and $E > 0$ is the total energy. Depending of whether particles are considered to be relativistic or not the energy $\mathcal{E}(p)$ of a particle having momentum $p \in \mathbb{R}^3$ is defined by

$$\mathcal{E}(p) = \mathcal{E}_{nr}(p) = \frac{|p|^2}{2m}, \tag{1.3}$$

for a non-relativistic particle, and by

$$\mathcal{E}(p) = \mathcal{E}_r(p) = \gamma mc^2, \quad \gamma = \sqrt{1 + \frac{|p|^2}{c^2m^2}}, \tag{1.4}$$

for a relativistic particle. The entropy H corresponds to the classical Boltzmann-Maxwell entropy (of non quantum particles) when $\tau = 0$, it corresponds to the Bose-Einstein entropy (of quantum particles of Bose type) when $\tau > 0$ (and for the sake of simplicity we will restrict ourself to $\tau = 1$, in the sequel) and it corresonds to the Fermi-Dirac entropy (of quantum particles of Fermi type) when $\tau < 0$ (and again, we only consider the case $\tau = -1$).

Considering one of the above entropies H and one of the above energies $\mathcal{E}$ we are therefore looking for a density function $\mathcal{G} \geq 0$ satisfying the moments constraint (1.2) and

$$H(\mathcal{G}) = \max_{g \text{ satisfying } (1.2)} H(g). \tag{1.5}$$

The above entropy maximisation problem is a very fundamental problem of statistical physic since its solution $\mathcal{G}$ corresponds to the microscopic momentum distribution of a gas of particles at the rest whose macroscopic observable mass, momentum and energy are N, P and E. The density distribution $\mathcal{G}$ is called the thermal equilibrium state. Out of rest, the evolution of the momentum gas distribution is usually discribed by a Boltzmann equation. The equilibrium state $\mathcal{G}$ is then (at least formally) a steady state to the associated Boltzmann equation. Moreover, any solution to the Boltzmann equation associated to an initial datum of macroscopic mass N, momentum P and energy E is expected to converge to the corresponding equilibrium state $\mathcal{G}$ in the large time asymptotic. For more details on this huge and difficult subject, we refer to [4], [22] and the many references therein for the classical Boltzmann equation, to [7], [18], [19] for the Fermi-Boltzmann equation, to [17], [11] for the Boltzmann equation associated to a gas of Bose particles and to [14], [8], [15], [1] for the relativistic Boltzmann equation. We also refer to [12] for a general mathematical presentation of the Boltzmann equation in a quantum and relativistic framework. A classical physical reference is [16].

A first simple and heuristic remark is that if $\bar{g}$ solves the entropy maximisation problem with constraint (1.2), there exists Lagrange multipliers $\mu \in \mathbb{R}$, $\beta^0 \in \mathbb{R}$ and $\beta \in \mathbb{R}^3$ such that

$$\big\langle \nabla H(\bar{g}), \varphi \big\rangle = \int_{\mathbb{R}^3} h'(\bar{g}) \varphi \,\mathrm{d}p = \big\langle \beta^0 \mathcal{E}(p) - \beta \cdot p - \mu, \varphi \big\rangle$$

for all φ, which implies

$$\ln(1 + \tau \bar{g}) - \ln \bar{g} = \beta^0 \mathcal{E}(p) - \beta \cdot p - \mu,$$

and in turn leads to

$$\bar{g}(p) = \frac{1}{\mathrm{e}^{\nu(p)} - \tau} \quad \text{with} \quad \nu(p) := \beta^0 \mathcal{E}(p) - \beta \cdot p - \mu. \tag{1.6}$$

The function $\bar{g}$ is called a *Maxwellian* when $\tau = 0$, a *Bose-Einstein distribution* when $\tau = 1$ and a *Fermi-Dirac distribution* when $\tau = -1$.

Let us consider for a moment the case $\tau = 0$, *i.e.* the classic (non-quantum non-relativistic) maximisation problem. In that case, the following result is known (and is almost trivial).

THEOREM 1. — *For any measurable function $\mathcal{G} \geq 0$ on $\mathbb{R}^3$ such that*

$$\int_{\mathbb{R}^3} \mathcal{G} \Big(1, p, \frac{|p|^2}{2} \Big) \,\mathrm{d}p = (N, P, E) \tag{1.7}$$

for some $N, E > 0$, $P \in \mathbb{R}^3$, the following assertions are equivalent:

(i) *$\mathcal{G}$ is the Maxwellian*

$$\mathcal{M}_{N,P,E} = \mathcal{M}[\rho, u, \Theta] = \frac{\rho}{(2\pi\Theta)^{3/2}} \exp\Big(- \frac{|p-u|^2}{2\Theta} \Big)$$

where (ρ, u, Θ) is uniquely determined by

$$N = \rho, \quad P = \rho u, \quad E = \frac{\rho}{2} \big(|u|^2 + 3\Theta \big);$$

(ii) *$\mathcal{G}$ is the solution of the maximisation problem*

$$H(\mathcal{G}) = \max \big\{ H(g) \,;\, g \text{ satisfies the moments constraint } (1.2) \big\},$$

where $H(g) = -\int_{\mathbb{R}^3} g \log g \,\mathrm{d}p$ stands for the classical entropy.

Our main result is the extension of Theorem 1 to the quantum non-relativistic and quantum relativistic framework, or in other words, we solve the maximisation problem (1.1)–(1.5) in the most general case. Before stating it, we would like to make some elementary remarks to convince the reader how different are the non quantum, the Bose and the Fermi cases.

On the one hand, the natural functional spaces to look for the density f are the spaces of distribution $f \geq 0$ such that the "physical" quantities are bounded:

$$\int_{\mathbb{R}^3} f\big(1+\mathcal{E}(p)\big)\,\mathrm{d}p < \infty \quad \text{and} \quad H(f) < \infty.$$

In the Fermi case where $\tau = -1$, $h(f) = +\infty$ if $f \notin [0,1]$ and so $H(f) < \infty$ provides a strong L^∞ bound on f. While in the Bose case, *i.e.* for $\tau = 1$, one has $h(f) \sim \ln f$ when $f \to \infty$, so that the entropy bound does not give any additional information than the moments bound. This provides very different conditions since we obtain:

$$f \in \begin{cases} L^1_s \cap L\log L & \text{in non quantum case, relativistic or not,} \\ L^1_s \cap L^\infty & \text{in the Fermi case, relativistic or not,} \\ L^1_s & \text{in the Bose case, relativistic or not,} \end{cases}$$

where

$$L^1_s = \Big\{ f \in L^1(\mathbb{R}^3)\,;\, \int_{\mathbb{R}^3} \big(1+|p|^s\big)\big|f(p)\big|\,\mathrm{d}p < \infty \} \Big\},$$

and $s = 2$ in the non relativistic case, $s = 1$ in the relativistic case.

On the other hand, it was already observed by Bose and Einstein (see [2], [9], [10]) that for systems of Bose particles in thermal equilibrium a careful analysis of the statistical physics of the problem leads to enlarge the class of steady distributions to include also the solutions containing a Dirac mass. More precisely, the class of Bose distributions $\overline{g}$ given by (1.6) has to be enlarged to the class of generalized Bose-Einstein relativistic distributions $\mathcal{B}$ defined by

$$\mathcal{B}(p) = b + \alpha\delta_{p_{MC}} = \frac{1}{\mathrm{e}^{\nu(p)} - 1} + \alpha\delta_{p_{MC}}, \quad \alpha \geq 0,\ p_{MC} \in \mathbb{R}^3. \tag{1.8}$$

Moreover, and still concerning the Bose case, considering any fixed vector $a \in \mathbb{R}^3$ and any approximation of the identity (φ_n) centered in a, it is shown in [3], see also Lemma 2.0, that for any $f \in L^1_2$ the quantity $H(f+\varphi_n)$ is well defined and

$$\lim N(f+\alpha\varphi_n) = N(f) + \alpha \quad \text{and} \quad \lim H(f+\varphi_n) = H(f) \quad \text{as } n \to \infty.$$

This indicates that the entropy H may be extended to nonnegative measures and that, moreover, the singular part of the measure does not contributes to the entropy. We will come back to this question in Section 3 below.

In the Fermi case, the strong uniform bound entailed by the entropy on the Fermi distributions leads to include in the family of Fermi steady states the so called-degenerate states. Therefore, one has to enlarge the class of Fermi-Dirac states given by (1.6) to the class of distributions (see for instance [21])

$$\mathcal{F}(p) = \frac{1}{\mathrm{e}^{\nu(p)} + 1} \quad \text{and} \quad \chi(p) = \mathbf{1}_{\{\beta^0 \mathcal{E}(p) - \beta\cdot p \leq 1\}}. \tag{1.9}$$

Our main result reads as follows.

Theorem 2. — *For every possible choice of* (N, P, E) *such that the set*

$$K = \big\{g\,;\, \textstyle\int_{\mathbb{R}^3} g(1, p, \mathcal{E}(p))\,\mathrm{d}p = (N, P, E)\big\},$$

is non empty, there exists a unique solution $\mathcal{G}$ *to the entropy maximisation problem*

$$\mathcal{G} \in K, \quad H(\mathcal{G}) = \max\big\{H(g)\,;\, g \in K\big\}.$$

Moreover, $\mathcal{G}$ *is the unique thermal equilibrium, i.e.* $\mathcal{G} = \overline{g}$ *given by* (1.6) *in the nonquantum case,* $\mathcal{G} = \mathcal{B}$ *given* (1.8) *in the Bose case, and* $\mathcal{G} = \mathcal{F}$ *given* (1.9) *in the Fermi case, satisfying the moments constraint* (1.2).

We refer to Theorems 2.1, 3.2 and 4.1 for more precise statements. It is of course looked as an evidence, in the physicist community, that equilibrium states (1.6), (1.8) and (1.9) are the solution to the associated entropy maximisation problem. Nevertheless, in the quantum case, we were not able to find a convincing proof of this fact. Indeed, it is not clear at all how to obtain an explicit expression of the thermal equilibrium $\mathcal{G}$ *(i.e.* values of β^0, β, $\mu, \dots$) as a function of the macropic quantities N, P, E. Our aim is to give here a rigorous and detailed proof of it.

The paper is organized as follows. In Section 2 we treat the relativistic non quantum case. In fact, this case was completely solved by R. Glassey and W.A. Strauss in [14], see also R. Glassey in [13] and [5]. However, we present here another proof, which uses in a crucial way, the Lorentz invariance and may be adapted to the quantum relativistic case.

We then deal with the Bose-Enstein gas in Section 3 and with the case of a Fermi-Dirac gas in Section 4. For each of these two kinds of gases, we first consider in detail the relativistic case and then briefly the non relativistic case, which is simplest since, by Galilean invariance, it can be reduced to $P = 0$.

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2. Relativistic non-quantum gas

In this section, we consider the Maxwell-Boltzmann entropy

$$H(g) = -\int_{\mathbb{R}^3} g \ln g \,\mathrm{d}p, \tag{2.1}$$