On the Connection of the Formulae for Entropy and Stationary Distribution

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Abstract

As it is well known in statistical physics the stationary distribution can be obtained by maximizing entropy. We show how one can reconstruct the formula for entropy knowing the formula for the stationary distribution. A general case is discussed and some concrete physical examples are considered.

1 Introduction

In this paper we distinguish entropy from other functionals of distribution functions. We show for a very general case that the entropy functional is the unique functional that is maximized by the corresponding stationary distribution function under constraints given by the invariants of the associated kinetic equations. This means we prove a generalization of the so called dual to Gibb's Lemma, see Mc Kean [6]. As we will see the unique reconstruction of entropy is only possible if the dimension of the space of invariants is more than one.

The physical examples we discuss are Maxwell-, Bose-Einstein-, and Fermi-Dirac distributions and constraints given by the invariants of the Boltzmann- respectively Uehling-Uhlenbeck equations, compare e.g. Balescu[1]. A counter example with only one collision invariant is given by the equations of neutron transport, see Case/Zweifel[4].

Our theorem is closely connected to the uniqueness of entropy as the only increasing functional of the Boltzmann equation, see Mc Kean [6] for the Kac-model of the Boltzmann equation and Waldmann [9] and Vedenyapin [8] for the case of the full Boltzmann equation.

The question is also becoming of interest in another context: In many papers 'spurious invariants' arise for discrete models of the Boltzmann equation and for lattice gases, see Cabannes [3], Bernardin [2]. The following theorems deal with analogs of 'spurious decreasing functionals' in a very general case.

verting Formula

Before stating our main result we introduce some notations. Let $\varphi_1(v), \ldots, \varphi_N(v)$ be continuous functions on $\mathbb{R}^k$, the invariants.
The mapping $S : \mathbb{R} \to (a,b) \subseteq \mathbb{R}^+$ is assumed to be differentiable with $S' > 0$.
$f^A_{stat}(v) := S(< A, \varphi(v) >)$ with $\varphi = (\varphi_1, \ldots, \varphi_N)$ and $A = (A_1, \ldots, A_N) \in \mathbb{R}^N$ is called stationary distribution. Here $< \cdot, \cdot >$ denotes the scalar product in $\mathbb{R}^N$.

Example: Let $N = 5, k = 3, \varphi_i = v_i, i = 1,2,3, \varphi_4 = |v|^2, \varphi_5 = 1$. With $S(x) = \exp(x)(1 + \Theta \exp(x))^{-1}$ we get for $\Theta = 0$ the Maxwell distribution, for $\Theta = -1$ the Bose-Einstein distribution and for $\Theta = 1$ the Fermi-Dirac distribution.

Consider the mapping $\phi(v,u) : \mathbb{R}^k \times (a,b) \to \mathbb{R}$. Let $\phi(v,u), \phi_u(v,u)$ and $\phi_{uu}(v,u)$ be continuous with respect to (v,u). Moreover the function $\phi(v, f^A_{stat}(v))$ is assumed to be integrable for every $A \in \mathbb{R}^N$. Denote by $M_{f^A_{stat}}$ the set of continuous functions coinciding with $f^A_{stat}(v)$ outside some ball, that is

$$\begin{aligned} M_{f^A_{stat}} &= \{ g \in \mathcal{C}(\mathbb{R}^k) | a < g(v) < b \quad \text{for all} \quad v \in \mathbb{R}^k \quad \text{and for some} \\ & \qquad R = R(g) > 0 \quad \text{there holds} \quad g(v) = f^A_{stat}(v) \quad \text{for every} \quad |v| > R \}. \end{aligned}$$

We are concerned with the uniqueness of functionals of the form $G(g) = \int \phi(v, g(v))dv$. The functional G is said to attain a maximum for the stationary distribution f^A_{stat}, if $\forall A \in \mathbb{R}^N$ and for all $g \in M_{f^A_{stat}}$ such that

$$\int [f^A_{stat}(v) - g(v)] \varphi_i(v) dv = 0, \; i = 1 \ldots N \tag{2.1}$$

there holds

$$G(f^A_{stat}) \geq G(g).$$

Condition A:

We assume that $\varphi_1, \ldots, \varphi_N$ are linear independent functions and for any $v \in \mathbb{R}^k$ there is an $i = i(v) \in \{1, \ldots, N\}$ s.t.

$$\varphi_i(v) \neq 0 \tag{2.2}$$

Our main result is stated in

Theorem 2.1 *Suppose that condition A holds and the number N of linear independent invariants is not less than 2. If $G(g) = \int \phi(v, g(v))dv$ attains a maximum for all $f^A_{stat}, A \in \mathbb{R}^N$, then there exists $b \leq 0$ and $c \in \mathbb{R}^N$, s.t.*

$$\frac{\partial \phi}{\partial u}(v,u) = bS^{-1}(u) + < c, \varphi(v) > . \tag{2.3}$$

$$\frac{\partial \phi}{\partial u}(v,u) = \varphi_1(v)\eta\left(\frac{S^{-1}(u)}{\varphi_1(v)}\right)$$

the functional $G(g) = \int \phi(v, g(v))dv$ *attains a maximum for all* $f^A_{stat}, A \in \mathbb{R}^N$. *Here* η *is an arbitrary monotone decreasing function. This means that in this case there is no uniqueness of the functional* $G(g)$.

Proof of 2.1:

We consider the case of two linear independent invariants, $\varphi = (\varphi_1, \varphi_2), N = 2$. In the general case $N \geq 2$ the proof is quite similar. We proceed in several single steps:

Step 1:
The necessary condition for the conditional extremum is that there exist Lagrange multipliers $\lambda_i \in \mathbb{R}, i = 1, 2$ s.t.

$$\int [\psi(v, f^A_{stat}(v)) - \sum_{i=1}^{2} \lambda_i \varphi_i(v)] h(v) dv = 0$$

where $\psi(v,u) = \phi_u(v,u)$ and $h(v)$ is arbitrary.
With $\lambda(A) = (\lambda_1(A), \lambda_2(A)) \in \mathbb{R}^2$, where $A = (A_1, A_2) \in \mathbb{R}^2$, the above yields

$$\psi(v, f^A_{stat}(v)) = < \lambda(A), \varphi(v) > . \tag{2.4}$$

Step 2:
Here we show that for any $v_0 \in \mathbb{R}^k$ one can find $v_1, v_2 \in \mathbb{R}^k$ and $\alpha_1, \alpha_2 \in \mathbb{R}$ with $\alpha_1 \neq 0 \neq \alpha_2$, s.t. the vectors $\varphi(v_1)$ and $\varphi(v_2)$ are linear independent and

$$\varphi(v_0) = \alpha_1 \varphi(v_1) + \alpha_2 \varphi(v_2). \tag{2.5}$$

First we prove the auxiliary statement that the span L of the set $\{x \in \mathbb{R}^2 | x = \varphi(v), v \in \mathbb{R}^k\}$ coincides with $\mathbb{R}^2$: It is obvious that the dimension of L is $1 \leq \dim L \leq 2$. Suppose $\dim L = 1$. Then there would exist $w_0 \in \mathbb{R}^k$ and a function $c(v) : \mathbb{R}^k \to \mathbb{R}$ s.t. $\varphi(v) = c(v)\varphi(w_0), \forall v \in \mathbb{R}^k$ with $\varphi(w_0) \neq 0$. Choose $\alpha_1, \alpha_2 \in \mathbb{R}$ such that $|\alpha| + |\alpha_2| \neq 0$ and $\alpha_1 \varphi_1(w_0) + \alpha_2 \varphi_2(w_0) = 0$. We get

$$\alpha_1 \varphi_1(v) + \alpha_2 \varphi_2(v) = c(v)(\alpha_1 \varphi_1(w_0) + \alpha_2 \varphi_2(w_0)) = 0.$$

This contradicts the linear independence of φ_1 and φ_2 and proves $\dim L = 2$.
The statement of step 2 can be shown in the following way: We take $v_0 \in \mathbb{R}^k$ arbitrary and find $v_1 \in \mathbb{R}^k$ s.t. the vectors $\varphi(v_0)$ and $\varphi(v_1)$ are linear independent. This is possible because $\dim L = 2$. It is sufficient to show that there exists $v_2 \in \mathbb{R}^k$ s.t.

$$\beta\varphi(v_0) \neq \varphi(v_2) \neq \gamma\varphi(v_1) \ \forall \beta, \gamma \in \mathbb{R} \tag{2.6}$$

$T_0 \cap T_1 = \emptyset$. Therefore there exists $v_2 \in \mathbb{R}^k$ s.t. $v_2 \notin T_0 \cup T_1$. This yields (2.6).

Step 3:
We take an arbitrary $v_0 \in \mathbb{R}^k$ and find $v_1, v_2 \in \mathbb{R}^k$ and $\alpha_1, \alpha_2 \in \mathbb{R}$ satisfying (2.5) as proven in Step 2. Introducing the functions $\psi_i, i = 0, 1, 2$ by

$$\psi_i(u) = \psi(v_i, S(u))$$

we show in this step that the following identity is true:

$$\alpha_1 \psi_1(z_1) + \alpha_2 \psi_2(z_2) = \psi_0(\alpha_1 z_1 + \alpha_2 z_2) \tag{2.7}$$

$\forall z_1, z_2 \in \mathbb{R}$.

Using (2.4) we get $\forall A \in \mathbb{R}^2$

$$\begin{aligned}
&\alpha_1 \psi_1(< A, \varphi(v_1) >) + \alpha_2 \psi_2(< A, \varphi(v_2) >) \\
&= \alpha_1 \psi(v_1, S(< A, \varphi(v_1) >)) + \alpha_2 \psi(v_2, S(< A, \varphi(v_2) >)) \\
&= \alpha_1 < \lambda(A), \varphi(v_1) > + \alpha_2 < \lambda(A), \varphi(v_2) > \\
&=< \lambda(A), \varphi(v_0) >= \psi(v_0, S(< A, \varphi(v_0) >)) \\
&= \psi_0(< A, \varphi(v_0) >) = \psi_0(\alpha_1 < A, \varphi(v_1) > + \alpha_2 < A, \varphi(v_2) >)
\end{aligned}$$

This yields already (2.7) as can be seen by the following argument: Because the vectors $\varphi(v_1), \varphi(v_2)$ are linear independent, the vector (z_1, z_2) with components $z_1 =< A, \varphi(v_1) >$, $z_2 =< A, \varphi(v_2) >$ takes all values in $\mathbb{R}^2$, while A takes all values in $\mathbb{R}^2$.

Step 4:
We show that the function $\psi(v, S(u))$ has the form

$$\psi(v, S(u)) = c_1(v)u + c_2(v) \tag{2.8}$$

$\forall v \in \mathbb{R}^k$ and all $u \in \mathbb{R}$.
$c_1(v)$ and $c_2(v)$ are some continuous functions on $\mathbb{R}^k$.
Setting first $z_1 = 0$,then $z_2 = 0$ and finally $z_1 = z_2 = 0$ in (2.7) we get the identities

$$\begin{aligned}
\psi_0(\alpha_2 z_2) &= \alpha_2 \psi_2(z_2) + \alpha_1 \psi_1(0) \qquad \forall z_2 \in \mathbb{R} \\
\psi_0(\alpha_1 z_1) &= \alpha_1 \psi_1(z_1) + \alpha_2 \psi_2(0) \qquad \forall z_1 \in \mathbb{R} \\
\psi_0(0) &= \alpha_1 \psi_1(0) + \alpha_2 \psi_2(0)
\end{aligned}$$

Adding these equalities and using (2.7) we obtain a functional equation for ψ_0 namely

$$\psi_0(\alpha_1 z_2) + \psi_0(\alpha_2 z_2) - \psi_0(0) = \psi_0(\alpha_1 z_1 + \alpha_2 z_2) \tag{2.9}$$
$$\forall z_1, z_2 \in \mathbb{R}$$

$$\psi_0(u) = \psi(v_0, S(u)) = c_1 u + c_2, \tag{2.10}$$

where c_1 and c_2 are some constants. Since $v_0 \in \mathbb{R}^k$ has been choosen arbitrary, we deduce from (2.10)

$$\psi(v, S(u)) = c_1(v)u + c_2(v) \quad \forall v \in \mathbb{R}^k,\ u \in \mathbb{R}.$$

The continuity of the functions c_1 and c_2 follows from the continuity of ψ and S.

Step 5:
We prove that $c_2(v)$ has the form

$$c_2(v) =< c, \varphi(v) >$$

where $c = (c_1, c_2) \in \mathbb{R}^2$ is some vector.
Substituting $u =< A, \varphi(v) >$ in (2.8) and taking (2.4) into account yields $\forall v \in \mathbb{R}^k, \forall A \in \mathbb{R}^2$

$$\begin{aligned} < \lambda(A), \varphi(v) > &= \psi(v, f^A_{stat}(v)) = \psi(v, S(< A, \varphi(v) >)) \\ &= c_1(v) < A, \varphi(v) > + c_2(v). \end{aligned}$$

This gives

$$< \lambda(A), \varphi(v) >= c_1(v) < A, \varphi(v) > + c_2(v) \tag{2.11}$$

$\forall v \in \mathbb{R}^k, A \in \mathbb{R}^2$. Setting $A = (0,0)$ we find $c_2(v) =< c, \varphi(v) >$ with $c = \lambda((0,0)) \in \mathbb{R}^2$.

Step 6:
We prove $c_1(v) \equiv b$, where b is a constant. Using the result of Step 5 in (2.11) we get

$$< (\lambda(A) - c),\ \varphi(v) >= c_1(v) < A, \varphi(v) > \tag{2.12}$$

$\forall v \in \mathbb{R}^k$ and $\forall A \in \mathbb{R}^2$.

Consider the sets

$$\begin{aligned} U_0 &= \{v | \varphi_1(v) \neq 0 \neq \varphi_2(v)\} \\ U_1 &= \{v | \varphi_1(v) = 0, \varphi_2(v) \neq 0\} \\ U_2 &= \{v | \varphi_1(v) \neq 0, \varphi_2(v) = 0\} \end{aligned}$$

Because of condition A we have $U_0 \cup U_1 \cup U_2 = \mathbb{R}^k$. Setting $A = (1,1)$ in (2.12) we have

$$c_1(v) = \lambda_2((1,1)) - c_2 \quad \forall v \in U_1 \tag{2.13}$$

$$c_1(v) = \lambda_1((1,1)) - c_1 \quad \forall v \in U_2 \tag{2.14}$$

$$c_1(v) = \alpha_1 + \alpha_2 f(v), \ \forall v \in U_0 \tag{2.15}$$

with $\alpha_1 = \lambda_1((1,0)) - c_1, \ \alpha_2 = \lambda_2((1,0)) - c_2$ and $f(v) = \frac{\varphi_2(v)}{\varphi_1(v)}$.

Setting $A = (0,1)$ in (2.12)

$$c_1(v) = \beta_1 \frac{1}{f(v)} + \beta_2 \quad \forall v \in U_0 \tag{2.16}$$

with $\beta_1 = \lambda_1((0,1)) - c_1, \ \beta_2 = \lambda_2((0,1)) - c_2$
Equating the right parts of (2.15) and (2.16) we derive that $f(v)$ satisfies

$$\alpha_2 f^2(v) + (\alpha_1 - \beta_2) f(v) - \beta_1 = 0 \quad \forall v \in U_0$$

Hence $f(v)$ is constant on U_0.

(2.13), (2.14) and (2.15) together with the continuity of $c_1(v)$ yield the statement of this step.

Step 7:
In Step 4-6 we have shown

$$\psi(v,u) = bS^{-1}(u) + < c, \varphi(v) > \tag{2.17}$$

What is left for the last step is to show $b \leq 0$: We consider the difference

$$\begin{aligned} G(g) - G(f^A_{stat}) &= \int [\phi(v, g(v)) - \phi(v, f^A_{stat}(v))] dv \\ &= \int \psi(v, f^A_{stat}(v)) [g(v) - f^A_{stat}(v)] dv \\ &+ \frac{1}{2} \int \frac{\partial \psi}{\partial u}(v, \xi(g(v), f^A_{stat}(v))) [g(v) - f^A_{stat}(v)]^2 dv \end{aligned} \tag{2.18}$$

The first integral in the right part vanishes because of (2.1) and (2.4). With (2.17) the second one has the form

$$b \int \frac{[g(v) - f^A_{stat}(v)]^2}{S'(S^{-1}(\xi(g(v), f^A_{stat}(v))))} dv$$

Since $G(g) \leq G(f^A_{stat})$ we have

$$b \int \frac{[g(v) - f^A_{stat}(v)]^2}{S'(S^{-1}(\xi(g(v), f^A_{stat}(v))))} dv \leq 0.$$

Because S' was assumed to be positiv $b \leq 0$ follows. The proof of Theorem 2.1 is complete.
■

Substitute $f_{stat}(v)$ in (2.18) and use $\psi(v,u) = \varphi_1(v)\eta\left(\frac{\cdots}{\varphi_1(v)}\right)$ where η is monotone de-
creasing.
We get

$$G(g) - G(f^A_{stat}) = \int \varphi_1(v)\eta(A)[g(v) - f^A_{stat}(v)]dv$$
$$+\frac{1}{2}\int \eta'\left(\frac{S^{-1}(\xi(g(v), f^A_{stat}(v)))}{\varphi_1(v)}\right)\frac{[g(v) - f^A_{stat}(v)]^2}{S'(S^{-1}(\xi(g(v), f^A_{stat}(v))))}dv$$

Again the first term an the right vanishes forall $g(v)$ satisfying (2.1). The second term is nonpositive because of $\eta' \leq 0$ and $S' > 0$.
Hence the functional G attains a maximum for $f^A_{stat}(v)$ and the proof is complete. ■

Remark:
We show here that condition A, especially (2.2), is essential for the proof of Theorem 2.1., namely that it cannot be replaced by the weaker one

$$\varphi(v) \neq 0 \quad \text{for almost all} \quad v \in \mathbb{R}^k.$$

We consider the following example: Choose $\varphi_1(v), \varphi_2(v)$ s.t.

$$\begin{aligned}
\varphi_1(v) &\neq 0 \neq \varphi_2(v) \quad \forall v \neq 0 \\
\varphi_1(0) &= 0 = \varphi_2(0) \\
\varphi_1(v) &= \varphi_2(v) \quad \forall v > 0 \\
\varphi_1(v) &= 2\varphi_2(v) \quad \forall v < 0
\end{aligned}$$

We show that the functional $G(g) = \int \phi(v, g(v))dv$ attains a maximum for

$$f^A_{stat}(v) = S(A_1\varphi_1(v) + A_2\varphi_2(v))$$

not only in the case when $\frac{\partial \phi}{\partial u}$ has the form (2.3), but also when

$$\frac{\partial \phi}{\partial u}(v,u) = \psi(v,u) = \begin{cases} 0 & v \geq 0 \\ \varphi_1(v)\eta\left(\frac{S^{-1}(u)}{\varphi_1(v)}\right) & v < 0 \end{cases}$$

where η is an arbitrary monotone decreasing function s.t. ϕ, ϕ_u and ϕ_{uu} are continuous.
Using (2.18) we get

$$G(g) - G(f^A_{stat}) = \int \psi(v, f^A_{stat}(v))[g(v) - f^A_{stat}(v)]dv$$
$$+\frac{1}{2}\int \frac{\partial \psi}{\partial u}(v, \xi(g(v), f^A_{stat}(v)))[g(v) - f^A_{stat}(v)]^2 dv$$

For all g satisfying (2.1) the first integral vanishes. This is true since

$$\psi(v, f^A_{stat}(v)) = <\lambda(A), \varphi(v)> \ \forall v \in \mathbb{R}, A \in \mathbb{R}^2$$

$$\lambda_1(A) = -\lambda_2(A) = 2\eta(A_1 + \frac{A_2}{2}).$$

The second integral is nonpositive because

$$\frac{\partial \psi}{\partial u} = \begin{cases} 0 & v > 0 \\ \eta'\left(\frac{S^{-1}(\xi(g(v), f^A_{stat}(v)))}{\varphi_1(v)}\right) \cdot \frac{1}{S'(S^{-1}(\xi(g(v), f^A_{stat}(v)))}, & v < 0 \end{cases}$$

is nonpositive. This proves that G attains a maximum for f^A_{stat} for all functionals G of the above form not only for those fulfilling (2.3).

3 Examples

The main examples are the equations of Boltzmann and Uehling Uhlenbeck . The collision invariants are the ones in the example at the beginning of section 2. Corresponding to the existence of 5 conservation laws of mass, momentum and energy we have

$$N = 5 \text{ and } \varphi_i = v_i,\ i = 1,2,3,\ \varphi_4 = |v|^2,\ \varphi_5 = 1,\ v \in \mathbb{R}^3.$$

The stationary distributions are

$$f^A_{stat,\Theta}(v) = S^\Theta(< A, \varphi(v) >)$$

with $A \in \mathbb{R}^5$ and $S^\Theta(x) = \exp(x)(1 + \Theta\exp(x))^{-1}$, where $\Theta = 0$ stands for Maxwell, -1 for Bose-Einstein and 1 for the Fermi-Dirac distribution. The usual form of these distributions is obtained by setting

$$A_i = \frac{u_i}{T},\ i = 1,2,3,\ A_4 = -\frac{1}{2T},$$

$$A_5 = -\frac{|u|^2}{2T} + \ln\left(\frac{\rho}{(2\pi T)^{\frac{3}{2}}}\right)$$

with $\rho, T \in \mathbb{R}^+, u \in \mathbb{R}^3$. For $\Theta = -1$,i.e. the Bose-Einstein case, ρ and T have to be restricted further by $\rho < (2\pi T)^{\frac{3}{2}}$. With Theorem 2.1 we get

Proposition 3.1 *If the functional* $G(g) = \int \phi(v, g(v))dv$ *attains a maximum for the stationary distributions* $f^{(\rho,u,T)}_{stat,\Theta}$ *with* ρ, u, T *as above, then:*

$$\begin{aligned} \phi(v,g) &= b[g\ln g + \Theta(1 - \Theta g)\ln(1 - \Theta g)] \\ &+ (\sum_{i=1}^{3} c_i v_i + c_4|v|^2 + c_5)g \\ &+ d(v) \end{aligned}$$

Here $b \le 0, c \in \mathbb{R}^5$ *is a constant vector and* d *an arbitrary function of* v.

An example with only one collision invariant is given by the neutron transport equation, a linear Boltzmann equation. v is restricted to a ball or sphere $B \subseteq \mathbb{R}^3$. There is only one collision invariant, $\varphi = \varphi_1 = 1$. This corresponds to the existence of just one conservation law, the conservation of mass. The stationary distribution is given by setting $S = Id$, i.e $f^\rho_{stat} = \rho, \rho \in \mathbb{R}^+$. According to Theorem 2.2 the functional $G(g) = \int\limits_B \phi(v, g(v))dv$ attains a maximum for all $f^\rho_{stat}, \rho \in \mathbb{R}^+$, if ϕ_u has the form

$$\phi_u(v,u) = \varphi(v)\eta\left(\frac{S^{-1}(u)}{\varphi(v)}\right) = \eta(u)$$

where η is an arbitrary monotone decreasing function. In other words: Any functional $G(g) = \int\limits_B \phi(v, g(v))dv$ with a concave function $\phi(v,u) = \phi(u)$ attains a maximum for $f^\rho_{stat}(v) = \rho, v \in B$ under the constraint

$$\int\limits_B [\rho - g(v)]dv = 0.$$

We remark that this is nothing but a restatement of Jensen's inequality.

Other examples are given by analogs of the Theorem proved above for discrete velocity models and lattice gases. For instance for the Carleman model we are in the situation of Theorem 2.2 but for the Broadwell model in the one of Theorem 2.1. This means that for the Carleman model 'spurious decreasing functionals' exist, see Godunov and Sultangazin [5]. The general theory of 'spurious decreasing functionals' and 'spurious invariants' for discrete models and lattice gases will be published.

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