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LOCAL SURROGATES OF THE MAXWELL HYPOTHESIS

Otto Moeschlin

Faculty of Mathematics and Computer Science
University of Hagen
58084 Hagen / Germany *otto.moeschlin@fernuni-hagen.de*

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1 Introduction

Generalizing the well-known Maxwell Hypothesis which characterizes in its original formulation the momentum distribution of a system of moving (and colliding) micro-constituents as a centred normal distribution, (its variance essentially being determined by the temperature), we arrive at a density function of the exponential type, its exponent being determined by the Hamiltonian of the system of micro-constituents as well by its temperature, the latter having the status of a specified parameter.
The Maxwell Hypothesis is a 'global' concept, it characterizes the equilibrium momentum distribution (of a system of moving molecules) on the whole momentum space.

Let the Hamiltonian H: $IU^N := IR^{2N} \to IR_+$ of a system of N micro-constituents with momenta $u^{(1)}, \ldots, u^{(N)}$ and $IU = IR^2$ as momentum space of the i-th micro – constituent be given by:

(1.1) $$H(u^{(1)}, \ldots, u^{(N)}) := \frac{1}{2}\sum_{j=1}^{N} \langle u^{(j)}, M^{-1}u^{(j)} \rangle$$ where

$\langle . , . \rangle$ denotes the standard scalar product on IR^2 and

(1.2) $$M := \begin{pmatrix} m1 & 0 \\ 0 & m2 \end{pmatrix}, \quad m1, m2 > 0$$

a positive definite and symmetric, here by reasons of simplicity, a diagonal mass matrix which also is not covered by Newtonian dynamics for the case of $m_1 \neq m_2$. This of course does not mean any limitation nor for the mathematical treatment nor for computer experimentation, but it allows more specific insights into the topic to be analyzed here.

The equilibrium momentum distribution

(1.3) $$P_{(T)} = \otimes_{j=1}^{N} N(0, M / k_B T)$$

at T being the temperature (of the system of micro-constituents) is given – according to the generalized Maxwell Hypothesis, c.f. *Moeschlin, Grycko 2006*, Section 2.3 – as the N^{th} power of the normal distribution

(1.4) $$N(0, M / k_B T)$$

where k_B denotes the Boltzmann constant.
Notice, the normal distribution $N(0, M / k_B T)$ on the meausurable space (IR^2, B^2) with the Borel σ-field B^2 has -- in case of $m_1 \neq m_2$ -- elliptical contours.(For reasons of simplicity σ-fields will not be mentioned more in the sequel.).
Moreover the empiric, i.e. estimated, momentum distribution of a system of micro-constituents with mass matrix M according to (1.2) indeed coincides with $P_{(T)}$, as can be shown by computer experimentation, cf. *Moeschlin, Grycko 2006* Chapter 7.

It is the merit of Ludwig Boltzmann to have introduced the model of moving and colliding micro-constituents (Boltzmann model, Boltzmann system), i.e. a model of mechanical dynamics to explain the phenomena of thermodynamics.
A momentum exchange is always initiated by a collision of (two) micro-constituents in the ortsraum, where the outcome of such a collision, i.e. the momentum exchange vector, is essentially determined by the momentum exchange direction, i.e. the difference of the positions of the colliding micro-constituents taken as unit vector. Thereby the moving and colliding micro-constituents might be seen as somewhat like a machine generating randomly these momentum exchange directions according to (a) probability law(s).

The questions to be treated here are: Can the momentum exchange concept be liberated from any mechanical dynamics? – e.g. can it be substituted by (a) probability law(s)? And, if yes, does the Maxwell Hypothesis (possibly in its generalized form) still hold true for an accordingely modified momentum exchange concept, liberated from any mechanical dynamics?

2 The set of all possible energy preserving momentum exchange vectors

Depending on the question to be treated it is more sensible not to see the momentum exchange direction as the normalized difference of the position-vectors of the colliding micro-constituents but to assume its polar angle φ as given. In this sense define the momentum exchange direction of the micro-constituents i and j with a specified polar angle φ by

(2.1) $$e^{(i,j)}_{\varphi} := (\cos\varphi, \sin\varphi)^t, \quad \varphi\in[0, 2\pi) =: I$$

According to principles of mechanics the momentum exchange vector of the micro-constituents i and j is determined by by the ansatz

(2.2) $$\begin{aligned} \underline{u}^{(i)} &= u^{(i)} + \xi_\varphi e^{(ij)}_\varphi \\ \underline{u}^{(j)} &= u^{(j)} - \xi_\varphi e^{(ij)}_\varphi \end{aligned}$$

where scalar ξ_φ is fixed by the condition of energy conservation, i.e. by

(2.3) $$H_0(u^{(i)}) + H_0(u^{(j)}) = H_0(\underline{u}^{(i)}) + H_0(\underline{u}^{(j)})$$

where $\underline{u}^{(i)}$ and $\underline{u}^{(j)}$ denote the momenta of micro-constituents i and j after the momentum exchange.

The (energy preserving) momentum exchange vector $a^{(ij)}_\varphi$. for the micro-constituents i and j with momentum exchange direction $e^{(ij)}_\varphi$ is determined as

(2.4) $$a^{(ij)}_\varphi := \xi_\varphi e^{(ij)}_\varphi .$$

When the momentum exchange direction and also the momentum exchange vector have to be understood as elements generated by the dynamics of the Boltzmann system we write

(2.5) $$e^{(ij)} \text{ instead of } e^{(ij)}_\varphi \text{ and } a^{(ij)} \text{ instead of } a^{(ij)}_\varphi .$$

Based on (2.4) the *set of all possible energy preserving momentum exchange vectors* is introduced as

(2.6) $$E^{(ij)} := \{ a^{(ij)}_\varphi \mid \varphi \in I\}.$$

3 The Uniform Distribution Hypothesis

By mathematical considerations it can be shown, that $E^{(ij)}$ is an ellipse in IR^2 whose points (y_1,y_2) satisfy the equation

$$(3.1) \qquad (y_1 - 1/2\ d_1^{(ij)})^2 / m_1 r_{(ij)}{}^2 + (y_2 - 1/2\ d_2^{(ij)})^2 / m_2 r_{(ij)}{}^2 = 1$$

with $(d_1^{(ij)}, d_2^{(ij)}) =: d(ij) =: u^{(i)} - u^{(j)}$ and $r_{(ij)} \in IR$.

Decisive for the present research is the Uniform Distribution Hypothesis (UDH) which states:

The momentum exchange vectors $a^{(ij)}$ generated by the dynamics of the Boltzmann system, here with mass matrix M according to (1.2), (but of course with any symmetric and positive definite mass matrix) follow a uniform probability distribution on the ellipse $E^{(ij)}$.

The proof of the UDH is given computer experimentally in a separate paper based on mathematical preparations, *Grycko, Moeschlin 2007*.

The UDH characterizes at certain time points the distribution of momentum exchange vectors of two colliding micro - constituents on the ellipses $E^{(ij)}$, in this sense we may speak of a 'local' concept also formulated as a probability law.. This gives raise to the question whether the UDH may be used to define an momentum exchange concept independent of any mechanical dynamics playing in the ortsraum of the micro - constituents

4 An Ortsraum Independent Momentum Exchange Concept (OIMEC)

The momentum status of a system of micro-constituents 1, … ,N, described by the vector

$$(4.1) \qquad (u^{(1)}, \dots ,u^{(k)}, \dots ,u^{(l)},\dots,u^{(N)})$$

is altered chronologically, i.e. step by step, according to the following rules:

1. Generate at any step a pair (k,l) of micro-constituents according to the uniform distribution on $IN_N \times IN_N$.
2. Generate a realization $\hat{a}^{(kl)}$ as omentum exchange vector of the micro - constituents according to the uniform probability distribution on the ellipse $E^{(kl)}$.
3. The new momentum status of the system of micro-constituents is given by

$$(4.2) \qquad (u^{(1)}, \dots u^{(k)} + \hat{a}^{(kl)} ,\dots,u^{(j)} - \hat{a}^{(kl)} ,\dots u^{(N)}).$$

The question to be cleared now is, does the OIMEC show the same momentum distribution as known for a Boltzmann system, i.e. does also the OIMEC fulfill the (generalized) Maxwell Hypothesis?
Notice, that the OIMEC is chronologically organized, i.e. step by step, but it does not depend on certain time intervals between the steps of alteration of the momentum status.

5 Statistical Analysis

The intention is to show that the empiric momentum distribution estimated directly by the momentum data of a sequence of momentum statii (4.1) from a computer experiment and collected in IR^2 coincides with the equilibrium momentum distribution, according to a

generalized Maxwell Hypothesis, i.e. $N(0, M / k_B T)$, cf.(1.4), which is a bivariate normal distribution with possibly an elliptical contour, (i.e. it is not necessarily more rotational symmetric,) where the covariance matrix is determined (estimated) based on the same momentum data.
This analysis is done according to the techniques developed in *Moeschlin, Grycko 2006,* Sections 1.6, 1.7 and 7.6.
To this end a linear subspaces L_τ of IR^2, $\tau \in [0°,360°)$ is introduced, projecting then the momentum data of IR^2 onto L_τ, $\tau \in [0°,360°)$. Using a kernel density estimator, (which is a tool from non-parametric statistics, estimating the graph of a density, cf. *Nadaraya 1989)*, we estimate the graph of the density of the projection of the empiric distribution on IR^2 onto L_τ to compare it with the projection of $N(0, M / k_B T)$ (equilibrium momentum distribution according to the generalized Maxwell Hypothesis) onto L_τ, which also is a normal distribution, its variance being estimated within the class of centred normal distributions on L_τ by the projected momentum data onto L_τ, for all $\tau \in [0°,360°)$. For details we refer to *Moeschlin, Grycko 200,* Chapter 7.
In case of statistical coincidence of the empiric and the equilibrium momentum distributions (according to the Maxwell Hypothesis) projected onto L_τ, for all $\tau \in [0°,360°)$, it follows by a theorem of Wold, cf. *Bilingsley 1986,* Theorem 29.4, p.397, that also the original distributions on IR^2 coincide.
Indeed, our computer experiments show that kernel density estimates generated by the momentum data projected onto L_τ approximate and coincide finally statistically with the projected equilibrium momentum distribution onto L_τ.,$\tau \in [0°,360°)$, this means that the OIMEC suffices the generalized Maxwell Hypothesis.

An another rather sensitive computer experiment to conduct, because it allows to quickly recognise incompatibilities, computes the temperature out of any projection of the momentum distribution on IR^2 onto L_τ, $0° \le \tau < 360°$.
Attaching to any $\tau \in [0°, 360°)$ the temperature T_τ computed for this τ one is led to a function $\tau \to T_\tau$, which has to be constant, as temperature is a scalar quantity.
Also this test is successfully passed in our research, which again confirms, that the OIMEC suffices the generalized Maxwell Hypothesis.

In this sense the Boltzmann system might be understood as a special implementation of the OIMEC.

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