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On the statistical fundamentals of modern thermofluiddynamics

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Dedicated to Prof. Dr.-Ing. Karl Stephan, Stuttgart, on the occasion of his seventieth birthday

Abstract — For a quantitative system theory, viz. the Gibbs–Falkian dynamics, it is shown that a special form of statistics exists which is inherently coupled to the model of systems comprised of particles. Derived via an interpolation problem, a partial differential equation is obtained exhibiting the structure of Schrödinger's wave equation. Depending on the type of particles assumed the equation is either linear or nonlinear. Nonlinearity and dissipation are inserted to the micro level of description by the respective Gibbs function of the system. These generalized Schrödinger equations which are given in extensive variables may be transformed to a space–time continuum in order to measure and control the system in regard. This is done by solving a system of linear equations. The resulting partial differential equations in time and spatial coordinates always are nonlinear. Similar to quantum mechanics, uncertainty relations may be constructed showing the principal lower bounds of the second moments for the extensive variables. As a mathematical concept, Gibbs–Falkian dynamics is not restricted to physics alone but has successfully been applied to other disciplines like, e.g., quantitative national economics. This holds as well for the presented statistical theory. However, in the context of this paper only the special case of thermofluiddynamics will be treated. © 2000 Éditions scientifiques et médicales Elsevier SAS

thermofluiddynamics / Gibbs function / Schrödinger equation / quantum theory / nonlinearity / dissipation

Nomenclature

A	parameter of the Maxwell–Boltzmann distribution
a_j	multiple of the increment of the jth variable
f	particle density in phase space
f_{MB}	Maxwell–Boltzmann distribution
$f_{\mathrm{MB,cont}}$	continuous form of Maxwell–Boltzmann distribution
H	dependent extensive variable
h	Planck's constant $= 6.6260755 \cdot 10^{-34}$ J·s
H_k	abbreviation for $\sqrt{\sum_{j=1,\, j\neq k}^{n} (\partial H/\partial X_j)^2}$
$\widehat{H}$	Gibbs function
$\hbar$	$h/2\pi$
k	degrees of freedom
N	number of particles
r	number of independent variables
$\boldsymbol{r}$	point vector
X_j	jth extensive variable
ΔX_j	inkrement of the jth independent variable X_j
Z	complex-valued function of the independent extensive variables

Greek symbols

α	parameter of the Maxwell–Boltzmann distribution
Γ	Gibbs Fundamental Relation
Ψ	complex-valued density of relative frequencies

Subscripts

j	variable counter
MB	belonging to the Maxwell–Boltzmann distribution

Mathematical symbols

e	Euler's constant
∇	nabla operator (gradient)
Δ	Laplace operator
i	imaginary unit
$\overline{(\ldots)}$	mean value of $(\ldots)$
$:=$	definition

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1. SUNDRY REMARKS ON GIBBS–FALKIAN DYNAMICS

Gibbs–Falkian dynamics, developed from Gibbsian thermostatics, has primarily been used as a unique and universal tool to describe thermodynamic phenomena. In recent work it has been extended to nearly any kind of physical discipline including problems from classical mechanics, relativity theory, and electromagnetic theory [1].

Furthermore, by stripping all physical contents the purely mathematical core of the theory is discovered: it is a mathematical recipe for the quantitative description of objects which may be characterized by their ability to exchange material or immaterial quantities with other objects of same or other kind.

Gibbs–Falkian dynamics rests on three primitive notions, viz. those of *variables*, *states* and *systems*. Here, variables are mathematical elements, i.e. functions, used to map quantities being exchanged between physical or economic objects, taken from the empirical reality into the set of real numbers. The description of the object in regard is complete by definition, if every *essential* quantity exchanged is mapped by a certain variable. It makes sense to choose variables that have the same meaning throughout the whole scientific discipline and, therefore, to term them *standard variables* or *generic quantities* (e.g., the output of a national economy, measured by the gross national product, is undoubtedly such a standard variable).

Due to their nature as functions, the generics may attain values that are real numbers. By fixing the values of the r-many generics for an object X_j, $j = 0, 1, \ldots, r$, simultaneously, the *state* of the object is determined.

The complete set $\boldsymbol{S}$ of all states of an object is called the *system*.

Hence, a system in the dynamic sense is nothing but a relation, viz. the *Gibbs Fundamental Relation* (GFR), between all the standard variables of the respective model or theory. Every information available on the object is contained in the GFR. Note that starting from this level of description all arguments only relate to the theoretical item "system", not to the real object being regarded. Assuming that the GFR may be solved with respect to at least one of the variables, a so-called *Massieu–Gibbs function* (MGF) is generated thereby. The special set of standard variables, as well as the variables themselves, making the MGF homogeneous of degree one are called *extensive*. This special MGF is the prominent *Gibbs function* (GF). Linear homogeneity of the GF in this context is not a mathematical necessity but a very useful arrangement: without any difficulties descriptions with MGFs being homogeneous of degrees unequal one are possible, even MGFs which are not homogeneous at all may be constructed. However, linearly homogeneous functions offer a lot of mathematical advantages which one would have to abandon in this case (for a detailed discussion of this topic see, e.g., [2, pp. 25–57]).

The set of extensive generics spans a $(r + 1)$-dimensional, abstract algebraic space, usually called "phase space" or "Gibbs space".

Let us now assume that such a GF exists. In general terms it reads:

$$H = \widehat{H}(X_1, X_2, \ldots, X_r) \tag{1}$$

H is the special quantity X_0 for which the GFR was resolved.

The choice of the generics $X_1, X_2, \ldots, X_r$ and H is the crucial point of the modeling process and strongly influences the validity and applicability of the theory in regard. Fortunately, there is a reliable method, viz. Callen's principle, at hand, that helps to select the complete set of essential quantities. In short, it states that for any physical principle (the so-called "symmetries") obeyed by the model at least one variable has to appear in the set. One example should suffice: for the simplest model of a one-phase one-component body-and-field system the GF reads

$$E = \widehat{E}(\boldsymbol{P}, \boldsymbol{r}, S, V, N) \tag{2}$$

where E is the total energy of the system, $\boldsymbol{P}$ its linear momentum, $\boldsymbol{r}$ is the displacement vector of the center of gravity in the inertial field, and S, V stand for the entropy, the volume of the body part of the system, and N for the number of particles this body is comprised of, respectively.

Conservation of total energy and the mass is represented by the variables E and N; the variables $\boldsymbol{P}$ and $\boldsymbol{r}$ assure the conservation of linear momentum. V is used to separate the material or body part of the system against the immaterial field while the entropy S opens the possibility to compose the system with others to a new (and larger) one or to decompose it into smaller subsystems. The two latter variables represent so-called "broken symmetries": no conservation laws exist for the entropy and the volume. Broken symmetries indicate higher symmetry states laying hidden in the mathematical background of the system. A detailed dicussion on the connection between systems, symmetries, and conservation laws is given in [3].

2. STATISTICS OF MULTI-PARTICLE SYSTEMS

To proceed to the statistical basis of GFD focus is now laid on a special class of systems: only those objects will be considered which consist of a sufficiently large but finite number of particles. The term "particles" here may refer to atoms, molecules or elementary particles for physical systems as well as to people or firms for economical applications. Because almost any real object may be regarded as consisting of particles a very broad range of systems is covered. The notion "sufficiently large" is fixed to the stability of the first moments of the generics. For unimodal distributions with finite standard deviations a lower bound for this number may be calculated, provided a limit for the acceptable change of the first moment is given. In Einstein's mechanics a "particle" is anticipated as the simultaneous transport of energy and linear momentum through the empty space (the "vacuum"). Comparing the mole volume and the volume that an atom occupies with respect to the number of atoms or molecules in a mole (Avogadro's number $N_A = 6.0225{\cdot}10^{23}$ particles per mole) one finds that fluids or even solid bodies nearly totally consist of empty space. Thus, the model of simultaneous energy–momentum transport which is basic for Gibbs–Falkian dynamics seems to be adequate for a realistic matter model. These particles should be distinguishable and may, therefore, be signed by an individual marker. Furthermore, an additional aspect is taken into account: *in reality* by no means it is possible to measure the value of a variable as a real number although the *theory* uses this set. Any real measurement will only result in rational numbers with a limited amount of decimals; for every extensive variable there exists an individual increment which is the lower bound for the exactness of the measurement of its values.

Hence, the phase space spanned by the extensive variables is divided into cells whose border length is given by the increments mentioned above (*figure 1*).

Making use of the extensivity of the generics a first conclusion will be drawn: the mass of the body plays the role of the homogeneity factor and may be calculated by multiplying the specific particle mass and the number of particles. Therefore, one finds that every particle of the object bears an individual part of the values of the generics and may, thus, be assigned to a specific cell characterized by the appropriate integer multiple of the increments.

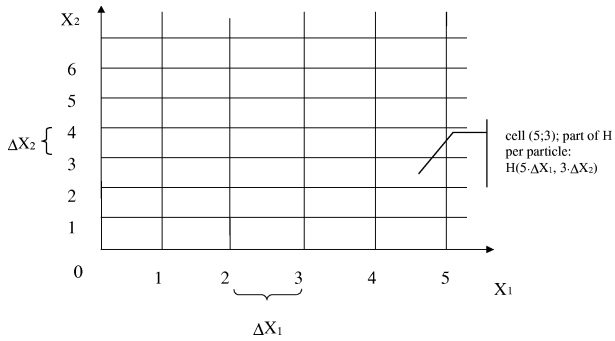

Figure 1. Example of a two-dimensional phase space divided into cells.

It is assumed that in principle a particle may access any cell of the phase space and that the number of particles in one cell is not limited.

Immediately the question arises which distribution of the particles over the cells is the most probable to appear for a fixed amount of H. The answer has first been given by Ludwig Boltzmann and is therefore called Maxwell–Boltzmann (MB) distribution. Its derivation may be looked up in any text book for statistical mechanics [4, 5] and will be neglected here. The result reads:

$$f_{\mathrm{dis}}(a_1\Delta X_1, a_2\Delta X_2, \ldots, a_r\Delta X_r) = A\,\mathrm{e}^{-\alpha H(a_1\Delta X_1, a_2\Delta X_2, \ldots, a_r\Delta X_r)} \tag{3}$$

For the kind of particles mentioned above the Maxwell–Boltzmann distribution f_{dis} is the most probable distribution. Note that the increments ΔX_j, $j = 1, 2, \ldots, r$, may by no means be set to zero because they appear as denominators (or arguments of a logarithm) during the derivation. Hence, the MB distribution is discrete and may not be treated by the tools of the calculus. It should be mentioned that the constant α is characteristic for the specific application.

At this point the next question arises: while the theory so far is only worked out for the phase space spanned by extensive variables, the control of systems requires statements valid for a space–time continuum. The transformation from an $(r + 1)$-dimensional phase space to spatial and time coordinates is done by differential equations; thus, the MB distribution has to be replaced by some steady function.

Boltzmann's solution to this problem was mathematically in error. He let the increments shrink to infinitely small quantities and hence obtained

$$f_{\mathrm{MB,cont}}(X_1, X_2, \ldots, X_r) = A\,\mathrm{e}^{-\alpha H(X_1, X_2, \ldots, X_r)} \tag{4}$$

which is the steady version of the MB distribution. The consequences of this procedure are the following:

- As mentioned above, the increments appear as denominators of a fraction or as arguments of a logarithm, respectively. Making them infinitely small (and zero in the limit) will cause the expression to be optimized to diverge. The complete optimization process, therefore, becomes invalid; in other words: $f_{\mathrm{MB,cont}}$ is not the solution to the problem of the most probable distribution in the phase space.
- Infinitely small increments would result in an arbitrarily large number of cells and, hence, in infinitely many particles. This is the typical chain of thought for continuum mechanics but not for systems with a distinct and finite particle number.

A way to find the correct answer becomes obvious when the task is reformulated: we need to have a steady function which is differentiable and for which we know the values at certain discrete points, viz. for the cells of the phase space.

From the mathematical point of view this is nothing else but an interpolation problem.

Three conditions for the interpolating function may be given.

First condition. At the corners of the cells of the phase space the interpolating function f_{cont} must have the same values as the discrete MB distribution f_{dis}:

$$f_{\mathrm{cont}}(a_1\Delta X_1, a_2\Delta X_2, \ldots, a_r\Delta X_r) = A\,\mathrm{e}^{-\alpha H(a_1\Delta X_1, a_2\Delta X_2, \ldots, a_r\Delta X_r)} \tag{5}$$

Because the derivatives of f_{cont} are needed in the interpolation process and f_{dis} and $f_{\mathrm{MB,cont}}$ have the same values at corners of the cells it makes sense to use $f_{\mathrm{MB,cont}}$ to determine the derivatives of f_{cont}.

Second condition. The new function f_{cont} has to have the same gradient as $f_{\mathrm{MB,cont}}$ at the corners of the cells:

$$\nabla f_{\mathrm{cont}}(a_1\Delta X_1, a_2\Delta X_2, \ldots, a_r\Delta X_r) = \nabla f_{\mathrm{MB,cont}}(a_1\Delta X_1, a_2\Delta X_2, \ldots, a_r\Delta X_r) \tag{6}$$

Obviously, the gradient of f_{dis} in the inner of the cells vanishes identically. This collides with the second condition, stating a nonzero gradient in the corners. The contradiction is solved by a

Third condition. In the inner of the cells, the *squared* gradient of f_{cont} has to vanish:

$$(\nabla f_{\mathrm{cont}})^2 \equiv 0 \quad \text{or} \quad \sum_{j=1}^{r}\left(\frac{\partial f_{\mathrm{cont}}}{\partial X_j}\right)^2 \equiv 0 \tag{7}$$

The third condition is the very crucial point of the interpolation procedure. Because a sum of positive nonzero real numbers cannot vanish identically, the only way to satisfy the third condition is to assume f_{cont} to be complex-valued (this explains the privileged role of the complex numbers in quantum theory). This is the price to be paid for changing from the discrete distribution f_{dis} to the continuous function f_{cont}.

Combining the three conditions together with formulae (3) and (4) as well as applying some algebra finally leads to a second-order linear partial differential equation for the complex-valued particle number related density function [6]

$$\Psi := \frac{f_{\mathrm{cont}}}{N} \tag{8}$$

which reads

$$\Delta\Psi + Z\Psi = 0 \tag{9}$$

The abbreviation Z is comprised of the derivatives of the GF H and the constant α:

$$Z := \alpha^2 (H_k)^2 \pm \mathrm{i}\alpha\nabla\cdot(H_k)$$
$$H_k := \sqrt{\sum_{\substack{j=1\\ j\neq k}}^{r}\left(\frac{\partial H}{\partial X_j}\right)^2} \tag{10}$$

i is the imaginary unit.

Equation (9) is called *generalized Schrödinger equation* (GSE) because it has the same mathematical structure as Schrödinger's renowned wave equation from quantum mechanics. However, it is based on a far more general theory and, therefore, is not restricted to physics at all; moreover, there are some essential differences between quantum mechanics and the theory presented here:

- Its underlying fundamentals are purely statistical; no reference is made to any kind of mass-point model, the related Hamilton theory, and the operator formalism. Nevertheless, there is some mathematical correspondence in structure and properties of the equations of both theories.
- It is noteworthy that there is no mathematical deduction of the Schrödinger equation from quantum mechanics given by this theory.
- Although equation (9) shows a linear structure, the theory is completely nonlinear as is indicated by equation (10) and — in contrast to quantum theory — allows irreversibility to be built in at particle level.

The complex-valued density function Ψ has no obvious meaning but analogous to quantum theory it can be shown that the product of Ψ and its complex conjugate Ψ^* has the properties of a probability density or a relative frequency. Hence, a second differential equation is implied for this product:

$$\Delta\left(\Psi\Psi^*\right) + 2Z_{\mathrm{Re}}\Psi\Psi^* = 0 \qquad (11)$$

It states that the real-valued product $\Psi\Psi^*$ obeys a differential condition which has the same structure as equation (9) for Ψ; Z_{Re} is the real part of the complex function Z.

By solving the differential equation (11) for appropriate initial and boundary conditions, the distribution in phase space for a system governed by the GF (1) is obtained.

For the product of Ψ and its conjugate has to obey the conditions for a density, the factor Z must be real-valued, in other words: its imaginary part has to be set to zero. (This corresponds to the mathematical condition from quantum theory that the respective operator has to be Hermitian.)

The resulting equation

$$\nabla\cdot(H_k) = \sum_{k=1}^{r}\frac{\partial}{\partial X_k}\sqrt{\sum_{j=1,\,j\neq k}^{r}\left(\frac{\partial H}{\partial X_j}\right)^2} \stackrel{!}{=} 0$$

$$\Leftrightarrow \sum_{k=1}^{r}\left[\frac{\displaystyle\sum_{j=1}^{r}\left(\frac{\partial H}{\partial X_j}\,\frac{\partial^2 H}{\partial X_j\partial X_k}\right) - \frac{\partial H}{\partial X_k}\,\frac{\partial^2 H}{\partial X_k^2}}{\sqrt{\displaystyle\sum_{j=1}^{r}\left(\frac{\partial H}{\partial X_j}\right)^2 - \left(\frac{\partial H}{\partial X_k}\right)^2}}\right] = 0 \qquad (12)$$

is an intricate nonlinear differential condition for the GF H. It assures the compatibility between the microscopic particle model and the phenomenological level of the system theory expressed by H. Equation (12) opens a way to solve the aggregation problem by restricting the macroscopic GF in such a way that it may be calculated as a sum of all individual parts of H carried by the particles comprising the system.

By now we only treated systems with particles that are distinguishable. The question arises what happens if we drop this premise and turn to other kinds of particles which may not be distinguished. In quantum theory, those particles are called fermionic or bosonic depending on the fact whether a cell in the phase space may contain only one particle or it is open for an arbitrary number of particles.

It is interesting that — by the same chain of thought as equation (9) has been derived — a new differential equation results which is now nonlinear and contains the solution of (9) as a reference distribution:

$$\Delta\Psi + \left[2\left(\frac{\Psi}{\Psi_{\mathrm{MB}}}\right)^2 - \frac{\Psi}{\Psi_{\mathrm{MB}}}\right]Z\Psi = 0 \qquad (13)$$

Equation (13) is called the *nonlinear generalized Schrödinger equation* (NLGSE) and is the most fundamental condition that can be found for the distribution of particles over the cells of a phase space, given a system characterized by its GF H.

3. FINITENESS AND THE LIMITS OF MEASUREMENT: THE GENERALIZED UNCERTAINTY RELATIONS

By the aid of the generalized Schrödinger equations, so-called *generalized uncertainty relations* may be obtained. Their derivation is straight forward and analogous to those of the classical ones which can be looked up in common text books of quantum mechanics [7].

They will be given here in their most general form (see [6, pp. 55–61]):

$$\overline{X_j^2}\cdot\overline{F_j^2} > \frac{1}{4\alpha^2(r-1)} \qquad (14)$$

where F_j is the marginal distribution of the jth variable, α is the constant from the MB distribution and r is the number of independent variables. $\overline{X_j^2}$ and $\overline{F_j^2}$ mark the second moment of X_j and F_j, respectively.

With the help of the uncertainty relations the limited exactness of any measurement may be calculated as far as sufficient data for the specific variable and its marginal distribution are available. By restricting the independent variables of the system to the "classical" ones, viz. the linear momentum $\boldsymbol{P}$ and the coordinates $\boldsymbol{r}$, Heisenberg's prominent uncertainty relation is obtained and α is related to Planck's constant. Other relevant examples may be looked up in the author's book mentioned above (cf. [6]).

4. TRANSFORMATION TO A SPACE–TIME CONTINUUM

As has been stated in section 2, the control of systems requires a description in a space–time continuum. Usually, this continuum is a synonym for the combination of

the linear Newton time from physics and an isotropic, homogenous three-dimensional space. Although this concept may be an adequate basis to treat with problems from classical physics, it does not hold for all applications in general. Modern theories like superstrings require spatial continua with more than three dimensions; some authors discuss the usefulness of an imaginary time. Nevertheless has the construction of these spaces be investigated under the aspect of the existence of conserved quantities induced by the mathematical properties of the calculus and the necessities of physical principles. An extensive discussion on the connection between some classes of continuous transformations and the existence of conserved quantities via Noether's theorem is given in [3].

In spite of these objections and for the sake of simplicity, let us stick to the traditional number of spatial coordinates combined with one time parameter.

Each generic is now perceived as a function of space and time:

$$\begin{aligned} X_j &= \widehat{X}_j(\boldsymbol{r}, t), \quad j = 1, 2, \ldots, r \\ H &= \widehat{H}(\boldsymbol{r}, t) \end{aligned} \tag{15}$$

Thus, the complex-valued interpolation function works in spatial and a time coordinate; the chain rule of the calculus then delivers

$$\frac{\partial \Psi}{\partial \boldsymbol{r}} = \sum_{j=1}^{r} \frac{\partial \Psi}{\partial X_j} \frac{\partial X_j}{\partial \boldsymbol{r}} \quad \text{and} \quad \frac{\partial \Psi}{\partial t} = \sum_{j=1}^{r} \frac{\partial \Psi}{\partial X_j} \frac{\partial X_j}{\partial t} \tag{16}$$

for the first and

$$\begin{aligned} \frac{\partial^2 \Psi}{\partial \boldsymbol{r}^2} &= \sum_{j=1}^{r} \sum_{k=1}^{r} \left[\frac{\partial^2 \Psi}{\partial X_j \partial X_k} \left(\frac{\partial X_j}{\partial \boldsymbol{r}} \cdot \frac{\partial X_k}{\partial \boldsymbol{r}} \right) \right] \\ &\quad - \sum_{j=1}^{r} \frac{\partial \Psi}{\partial X_j} \frac{\partial^2 X_j}{\partial \boldsymbol{r}^2} \\ \frac{\partial^2 \Psi}{\partial t^2} &= \sum_{j=1}^{r} \sum_{k=1}^{r} \left[\frac{\partial^2 \Psi}{\partial X_j \partial X_k} \frac{\partial X_j}{\partial t} \frac{\partial X_k}{\partial t} \right] \\ &\quad - \sum_{j=1}^{r} \frac{\partial \Psi}{\partial X_j} \frac{\partial^2 X_j}{\partial t^2} \end{aligned} \tag{17}$$

for the second-order derivatives.

Obviously, this is a system of linear equations for the derivatives of the complex-valued interpolation function with respect to the extensive generics. Solving this system and inserting its solution in the differential equations (9) or (13), respectively, changes them to equations in space and time as well.

As far as we have four coordinates (three spatial and one time) and r-many generics, the system has k-many degrees of freedom with

$$k := \frac{1}{2}\left(r^2 + 3r - 8\right) \tag{18}$$

Even for a GF with only two independent variables k is equal to 1; k increases rapidly with the number of generics (as can easily be calculated, k is equal to 5 for $r = 3$).

This gives rise to the following statements:

- The transformation from phase space to parameter space is not unique. To achieve a unique solution, additional conditions, e.g., specific conservation laws, process restrictions, etc. have to be applied.
- Thus, phase space descriptions are far more general than those in the parameter space. This is true for all disciplines of physics as far as the method of Gibbs–Falkian dynamics may be applied. Therefore, the respective theories should be based on the concept of phase space variables.
- Theories derived from measurements done in the parameter space are incomplete; they are only special cases produced by specific process realizations. They cannot be transformed to the respective phase space theories because the connections are only relational.

5. CONCLUSIONS

For the concept of Gibbs–Falkian dynamics the statistical foundations of particle-based systems have been derived showing that there is a specific kind of statistics for GFD. It could be shown that for the discrete distribution of the particles in the phase space a complex-valued interpolation function exists which may be transformed to a function in space and time by means of the calculus. This interpolation function is the solution of a second-order partial differential equation which exhibits the structure of a wave equation and is either linear or nonlinear, depending on the type of particle model used. Inserting the Gibbs function of body-field systems into the generalized Schrödinger equations it can be shown how the phenomenological aspects like irreversibility and nonlinearity enter the particle level of the description. On the other hand, a condition is given restricting the GF and connecting the statistical and the macro level.

Similar to quantum theory, from the differential equations generalized uncertainty relations may be derived.

By the aid of these relations lower bounds for the measurement errors of the extensive variables may be given.

Finally, the transformation from phase space to parameter space has been performed by solving a specific system of linear equations. The solution of this system is not unique and has to be restricted by particular conditions for the process realization. Thus, the generality of the phase-space concept could be shown.

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