

# Derivation of the Schrödinger equation II: Boltzmann's entropy

Derivação da equação de Schrödinger II: a entropia de Boltzmann

Olavo L. da Silva Filho<sup>1</sup>, Marcello Ferreira<sup>\*1</sup>

<sup>1</sup>Universidade de Brasília, Instituto de Física, Centro Internacional de Física, Brasília, DF, Brasil.

Received on June 11, 2024. Revised on July 09, 2024. Accepted on July 19, 2024.

In a previous paper, we have mathematically derived the Schrödinger equation using the construct of a Characteristic Function. We have shown that this derivation has a great number of consequences and may help to understand what Quantum Mechanics is really about. In this paper, we present another axiomatic mathematical derivation based on the construct of Boltzmann's entropy. We also show how these two derivations are mathematically connected and obtain, from this, the positive definite phase space probability distribution function. This probability distribution function is shown to be the only one that reproduces the Schrödinger equation and maximizes entropy, while minimizing the energy. Bohmian Mechanics is considered and reinterpreted from the perspective of the mathematical results of the present approach. Some examples are worked out to give teachers interested in using this material in their classrooms some concreteness.

**Keywords:** Bohmian Mechanics, Entropy, Schrödinger equation, Mathematical derivation, Teaching of Quantum Mechanics.

Em um artigo anterior, derivamos matematicamente a equação de Schrödinger usando como construto a "Função Característica". Mostramos que esta derivação tem um grande número de consequências importantes e pode ajudar a compreender do que realmente trata a Mecânica Quântica. Neste artigo, apresentamos outra derivação matemática axiomática baseada no construto "entropia de Boltzmann". Mostramos também como essas duas derivações estão matematicamente conectadas e obtemos, a partir disso, a função de distribuição de probabilidade positivo – definida no espaço de fase. Esta função de distribuição de probabilidade mostra-se como a única capaz de reproduzir a equação de Schrödinger e maximizar a entropia, ao mesmo tempo que minimiza a energia. A Mecânica Bohmiana é considerada e reinterpretada a partir da perspectiva desenvolvida nesta abordagem a partir dos resultados matemáticos. Alguns exemplos são elaborados para dar alguma concretude aos professores interessados em utilizar este material em suas salas de aula.

**Palavras-chave:** Mecânica Bohmiana, Entropia, Equação de Schrödinger, Derivação matemática, Ensino de Mecânica Quântica.

## 1. Introduction

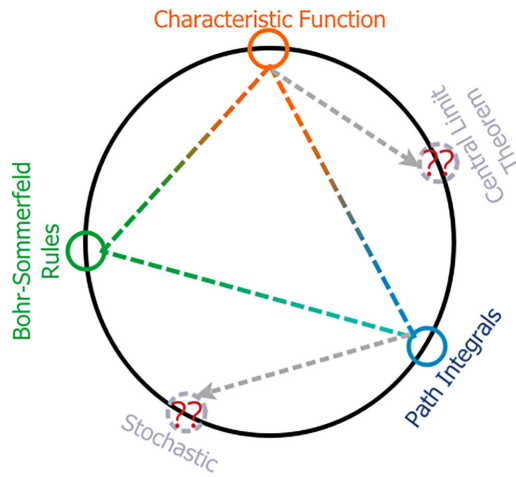
In paper I of this series [1], a mathematical method to derive the Schrödinger equation was presented. The method is based on the characteristic function construct – a fairly usual concept of Statistics in general. We showed the power of adopting an axiomatic approach by presenting other important results related to the process of quantization. The approach is based on two axioms and is mathematically quite direct. That paper followed lines similar to those adopted in [2, 3], in which we tried to make a didactic transposition of topics related to the foundations of Quantum Mechanics.

At this point, one may ask why trying to derive the Schrödinger equation by other ways, if the one already presented is so rich of results and mathematically direct? The point is that each formalism used to make quantization is based upon different formal constructs and

give us ways of seeing the semantics of the field in different, but interconnected ways. This is, thus, a quite secure and careful way to address the problem of the interpretation of Quantum Mechanics, that shows itself to be quite complex since its proposition in terms of the Schrödinger equation, and even more to students initiating their understanding of the topic.

For instance, Feynman's approach works with the notion of *trajectories* and scratches the idea of a stochastic behavior, when it presents the mathematical fact that one may look at the formalism of the theory by a sort of *summing over an infinite set of trajectories* – these trajectories, with some stretch at least up to this point, may be connected to stochastic realizations of the system dynamics. However, this is nothing but a suggestion that *must* be clarified by other quantization methods, using constructs that are better fit to these notions. On the other hand, the characteristic function derivation gives us a glimpse that the Central Limit Theorem may play a central role in Quantum Mechanics. These two results

\*Correspondence email address: marcellof@unb.br



**Figure 1:** Formal connections already made (in color) and some connections scratched upon (in gray).

must be mathematically derived, if we want a sound basis for Quantum Mechanics – in particular regarding its interpretation. We thus have, up to now, made the mathematical interconnections shown in Figure 1.

The construct of the present paper is Boltzmann's entropy, known by us from our studies in the field of Thermodynamics. Again, this is a concept closely related to that of fluctuations. Thus, if we succeed in making this derivation and if we accomplish to show the mathematical equivalence between it and the characteristic function derivation (and, thus, also Feynman's path integral approach etc.), the use of the notion of fluctuation in the interpretation of the theory would begin to be justified.

As a formal result of the present derivation, we will show how these two approaches together help us finding a phase space distribution function that represents any phenomenon of Quantum Mechanics. As the reader will see, this distribution is positive definite and gives the correct quantum mechanical results whenever we calculate average values in the usual classical statistical way. We show this by applying the formalism to the harmonic oscillator and the hydrogen atom as examples.

The paper is organized in the following manner: in the second section we present the derivation, which is based on only two axioms, as was the case with the characteristic function derivation. In the third section we show how the present entropy derivation is connected to the characteristic function derivation of the previous paper. Section four will be devoted to the important issue of deriving the phase space probability density function. Section five will then show that the present approach can be used to understand, in a deeper way, Bohm's "hidden variables" approach (but in statistical terms, without the notion of "hidden variables"). To make the present approach as concrete as possible, we present two examples of the phase space probability density function in section six. In section seven, we

will show that the derived phase space probability density function indeed satisfies the first axiom of the characteristic function derivation – and how it does that. Section eight will be devoted to show that the phase space probability density function obtained is the only one that maximizes the phase space entropy. The last section is then devoted to our conclusions.

## 2. The Derivation

We begin, as in the previous paper [1], presenting the postulates of the derivation. Again, we need only two axioms [4]:

**Axiom 1** For an isolated system, the joint phase-space probability density function related to any Quantum Mechanical phenomenon obeys the momentum integrated Liouville equation as

$$\int_{-\infty}^{\infty} \frac{dF(q, p; t)}{dt} dp = 0; \int_{-\infty}^{\infty} p \frac{dF(q, p; t)}{dt} dp = 0, \quad (1)$$

**Axiom 2** The product of the variances of the momenta and the positions of a physical process, calculated at each point  $q$  of the configuration space, must satisfy

$$\langle \delta p(q; t)^2 \rangle \langle \delta q(q; t)^2 \rangle = \frac{\hbar^2}{4}. \quad (2)$$

It is important to understand what this last equation is saying, though. We say that  $p$  alone (and not  $p(q; t)$ ) is the variable that, by quantization turns into the operator  $\hat{p}$ , while  $\langle \delta p(q)^2 \rangle$  is the momentum fluctuation over a fiber on phase space labelled by  $q$ , that is, parallel to the momentum axis, with an analogous interpretation for  $\langle \delta q(q; t)^2 \rangle$ .

Before developing the derivation of the Schrödinger equation, it is important to stress that we are not saying, in Axiom 1, that the phase space probability density function  $F(q, p; t)$  must be a solution of the Liouville equation. On the contrary, in what follows, our formal developments will show clearly that this is not the case (except for the ground state of the Harmonic Oscillator). We are requesting that only the first two momentum statistical moments are given by the constraints in (1). Indeed, the first equation in (1) represents solely the continuity equation, which we know to be valid within Quantum Mechanics. The second equation in (1) is related to energy conservation, which is also a property of Quantum Mechanical systems, in general. These are the only demands put forward by Axiom 1. Moreover, the first axiom is completely general and can encompass many statistical physical systems which present conservation of probability and energy. What Axiom II does is precisely specify that, from all those systems, only those satisfying that condition should be considered.

We now show that these two axioms *alone* allow us to mathematically derive the Schrödinger equation in a quantization process, as explained in [1]. Much of the developments here follow quite closely the usual approach of classical kinetic theory[5].

The Liouville equation can be written as

$$\frac{\partial F(q, p; t)}{\partial t} + \frac{p}{m} \frac{\partial F(q, p; t)}{\partial q} - \frac{\partial V(q)}{\partial q} \frac{\partial F(q, p; t)}{\partial p} = 0,$$

and we can immediately integrate it with respect to  $p$  and use the definitions

$$\begin{aligned} \int F(q, p; t) dp &= \rho(q; t); \\ \int pF(q, p; t) dp &= p(q; t)\rho(q; t) \end{aligned}, \tag{3}$$

where  $\rho(q; t)$  is the probability density upon configuration space, and the product  $p(q; t)\rho(q; t)$  is the momentum density average, also defined upon configuration space. We arrive at the equation

$$\frac{\partial \rho(q; t)}{\partial t} + \frac{\partial}{\partial q} \left[ \frac{p(q; t)}{m} \rho(q; t) \right] = 0, \tag{4}$$

which is clearly a continuity equation for the probability density defined upon the configuration space. This, therefore, gives us a very direct interpretation of the probability current that one finds in the usual approach that *begins* with the Schrödinger equation.

This is our first result that will be compared with the formal derivation of paper I. The application of the second constraint in axiom 1, which involves the use of axiom 2, is, however, more involved.

Indeed, we may now multiply the Liouville equation by  $p$  and define, in a way parallel to previous ones in (3), the second order momentum statistical moment as

$$\int p^2 F(q, p; t) dp = M_2(q; t). \tag{5}$$

We get the equation

$$\frac{\partial}{\partial t} [\rho(q; t)p(q; t)] + \frac{1}{m} \frac{\partial M_2(q; t)}{\partial q} + \frac{\partial V(q)}{\partial q} \rho(q; t) = 0. \tag{6}$$

Using (4) into this last equation, we find, after some straightforward calculations, the expression

$$\begin{aligned} \frac{1}{m} \frac{\partial}{\partial q} [M_2(q; t) - p^2(q; t)\rho(q; t)] \\ + \rho(q; t) \left[ \frac{\partial p(q; t)}{\partial t} + \frac{\partial}{\partial q} \left( \frac{p^2(q; t)}{2m} \right) + \frac{\partial V(q)}{\partial q} \right] = 0. \end{aligned} \tag{7}$$

The first term of the previous expression may be written as

$$\begin{aligned} M_2(q; t) - p^2(q; t)\rho(q; t) \\ = \int [p^2 - p^2(q; t)] F(q, p; t) dp \\ = \int [p - p(q; t)]^2 F(q, p; t) dp. \end{aligned}$$

From the definitions in (3) and (5), we may also define the variance density of the variable  $p$  on each point of the configuration space, since integration is being made upon only the momentum variable, as

$$\langle \delta p(q; t)^2 \rangle \rho(q; t) = \int [p - p(q; t)]^2 F(q, p; t) dp. \tag{8}$$

At this point, we have not used the second axiom yet – it will be necessary precisely to allow us to find the expression for  $\langle \delta p(q; t)^2 \rangle$  in terms of the probability density function  $\rho(q; t)$ . This is the point at which Boltzmann’s entropy comes into play.

Thus, consider the *entropy*  $\mathfrak{S}(q; t)$  defined upon the configuration space in such a way that the equal *a priori* probability postulate grants us that (see [25], pp. 290, 509)

$$\rho(q; t) = \exp \left[ \frac{\mathfrak{S}(q; t)}{k_B} \right],$$

where  $k_B$  is Boltzmann’s constant. We now make the system to fluctuate around  $q$  by an amount  $\delta q$  in such a way that we have

$$\begin{aligned} \rho(q, \delta q; t) = \rho(q + \delta q; t) = \rho(q; t) \\ \times e \left[ \frac{1}{k_B} \left( \frac{\partial \mathfrak{S}(q + \delta q; t)}{\partial q} \right)_{\delta q=0} \delta q + \frac{1}{2k_B} \left( \frac{\partial^2 \mathfrak{S}(q + \delta q; t)}{\partial q^2} \right)_{\delta q=0} \delta q^2 \right], \end{aligned} \tag{9}$$

meaning that the perturbed  $\rho(q, \delta q; t)$  is a *Gaussian function* and is related to the probability of having a fluctuation  $\Delta\rho$  in the probability density function that may be different for different points  $q$  in the configuration space (this method of analysis has nothing new and was introduced by Einstein and Smoluchovsky; see [6], p. 172; see also [7], pp. 288-291). Note that we develop the expression *up to second order* in  $\delta q$  (which begins to show the deep connection with the derivation made in paper I [1] – and, again, with the Central Limit Theorem).

Thus, it is obvious that

$$\begin{aligned} \langle \delta q(q; t)^2 \rangle = \frac{\int_{-\infty}^{+\infty} (\delta q)^2 \exp(\beta \delta q - \gamma \delta q^2) d(\delta q)}{\int_{-\infty}^{+\infty} \exp(\beta \delta q - \gamma \delta q^2) d(\delta q)} \\ - \left( \frac{\int_{-\infty}^{+\infty} \delta q \exp(\beta \delta q - \gamma \delta q^2) d(\delta q)}{\int_{-\infty}^{+\infty} \exp(\beta \delta q - \gamma \delta q^2) d(\delta q)} \right)^2, \end{aligned}$$

where we put

$$\gamma = -\frac{1}{2k_B} \left( \frac{\partial^2 \mathfrak{S}(q; t)}{\partial q^2} \right)_0, \quad \beta = -\frac{1}{k_B} \left( \frac{\partial \mathfrak{S}}{\partial q} \right)_0.$$

A simple calculation of the integral shows that

$$\langle \delta q(q; t)^2 \rangle = \frac{1}{2\gamma} = -\left( \frac{\partial^2 \ln(q; t)}{\partial q^2} \right)^{-1}.$$

Note that we were looking for an expression for

$$\langle \delta p(q; t)^2 \rangle,$$

but ended up with an expression for  $\langle \delta q(q; t)^2 \rangle$ . In principle, there is no relation among these dispersions, and it is axiom 2 that brings about this relation, which may be thought as the main feature of Quantum Mechanics<sup>1</sup>.

Indeed, the content of the second axiom (and of Quantum Mechanics) allows us to write

$$\langle \delta p(q; t)^2 \rangle = -\frac{\hbar^2}{4} \frac{\partial^2 \ln \rho(q; t)}{\partial q^2},$$

and thus (see [41] p. 120 or [42])

$$\langle \delta p(q; t)^2 \rangle \rho(q; t) = -\frac{\hbar^2}{4} \rho(q; t) \frac{\partial^2 \ln \rho(q; t)}{\partial q^2}. \quad (10)$$

Substituting this last expression into (7) and writing, as in the derivation of paper I,

$$\rho(q; t) = R(q; t)^2; \quad p(q; t) = \frac{\partial S(q; t)}{\partial q}, \quad (11)$$

we find

$$\frac{\partial S}{\partial t} + \frac{1}{2m} \left( \frac{\partial S}{\partial q} \right)^2 + V(q) - \frac{\hbar^2}{2mR(q; t)} \frac{\partial^2 R}{\partial q^2} = 0. \quad (12)$$

Equations (4) and (12) were already shown in paper I to be equivalent to the Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial q^2} + V(q)\psi(q; t) = i\hbar \frac{\partial \psi(q; t)}{\partial t},$$

if we put

$$\psi(q; t) = R(q; t) \exp \left[ \frac{i}{\hbar} S(q; t) \right]. \quad (13)$$

Thus, the two axioms of this section also allow us to mathematically derive the Schrödinger equation.

From the previous calculations, we may hunch that *there must be* a relation between the derivation of paper I and the present one. This can be mathematically shown and we prove it in the next section.

### 3. Connections with the Characteristic Function Derivation

The characteristic function derivation of paper I used the expression

$$Z(q, \delta q; t) = \int F(q, p; t) \exp \left( \frac{i}{\hbar} p \delta q \right) dp, \quad (14)$$

<sup>1</sup> We will show that axiom 2, as expected, gives Heisenberg's relations as a formal consequence.

which implies that

$$\rho(q; t) = \lim_{\delta q \rightarrow 0} Z(q, \delta q; t)$$

$$p(q; t)\rho(q; t) = \lim_{\delta q \rightarrow 0} -i\hbar \frac{\partial Z(q, \delta q; t)}{\partial(\delta q)},$$

and

$$\int p^2 F(q, p; t) dp = \lim_{\delta q \rightarrow 0} -\hbar^2 \frac{\partial^2 Z(q, \delta q; t)}{\partial(\delta q)^2}.$$

Then, (8) becomes

$$\begin{aligned} & \langle \delta p(q; t)^2 \rangle \rho(q; t) \\ &= \lim_{\delta q \rightarrow 0} \left[ -\hbar^2 \frac{\partial^2 Z(q, \delta q; t)}{\partial(\delta q)^2} + \hbar^2 \left( \frac{\partial Z(q, \delta q; t)}{\partial(\delta q)} \right)^2 \right], \end{aligned}$$

which may be rearranged as

$$\begin{aligned} & \langle \delta p(q; t)^2 \rangle \rho(q; t) \\ &= -\hbar^2 \lim_{\delta q \rightarrow 0} Z(q, \delta q; t) \frac{\partial^2 \ln Z(q, \delta q; t)}{\partial(\delta q)^2}. \end{aligned}$$

It thus remains for us to calculate the explicit appearance of this expression and to show that it is equivalent to (10).

We may expand the exponential in (14) to write the characteristic function, up to second order in  $\delta q$ , as

$$\begin{aligned} Z(q, \delta q; t) &= \int F(q, p; t) dp + \frac{i\delta q}{\hbar} \int pF(q, p; t) dp \\ &\quad - \frac{(\delta q)^2}{2\hbar^2} \int p^2 F(q, p; t) dp \end{aligned}$$

and using (3) and (5) we rewrite it as

$$\begin{aligned} Z(q, \delta q; t) &= \rho(q; t) + \frac{i\delta q}{\hbar} p(q; t)\rho(q; t) \\ &\quad - \frac{(\delta q)^2}{2\hbar^2} M_2(q; t) + o(\delta q^3). \quad (15) \end{aligned}$$

The left-hand side, on the other hand, has to be written as

$$Z(q, \delta q; t) = \psi^* \left( q - \frac{\delta q}{2}; t \right) \psi \left( q + \frac{\delta q}{2}; t \right)$$

and using (13) we find, up to second order in the infinitesimal parameter  $\delta q$ , the expression (see paper I)

$$\begin{aligned} & Z(q, \delta q; t) \\ &= \left\{ R(q, t)^2 + \left( \frac{\delta q}{2} \right)^2 \left[ R(q; t) \frac{\partial^2 R}{\partial q^2} - \left( \frac{\partial R}{\partial q} \right)^2 \right] \right\} \\ &\quad \exp \left( \frac{i\delta q}{\hbar} \frac{\partial S}{\partial q} \right), \end{aligned}$$

or, explicitly,

$$Z(q, \delta q; t) = R(q; t)^2 + \frac{i\delta q}{\hbar} R(q; t)^2 \frac{\partial S(q; t)}{\partial q} + \frac{(\delta q)^2}{2} \left[ \frac{1}{4} R(q; t)^2 \frac{\partial^2 \ln R(q; t)^2}{\partial q^2} - \frac{R(q; t)^2}{\hbar^2} \left( \frac{\partial S(q; t)}{\partial q} \right)^2 \right]. \tag{16}$$

Comparison of (15) with (16) shows that

$$\rho(q; t) = R(q; t)^2; \quad p(q; t) = \frac{\partial S(q; t)}{\partial q}, \tag{17}$$

as in (11), and

$$M_2(q; t) = -\frac{\hbar^2}{4} \rho(q; t) \frac{\partial^2 \ln \rho(q; t)}{\partial q^2} + p(q; t)^2 \rho(q; t).$$

Now, using (15), we can write (up to second order)

$$Z(q, \delta q; t) = \rho(q; t) \left[ 1 + \frac{i\delta q}{\hbar} p(q; t) + \frac{(\delta q)^2}{2} \left( \frac{1}{4} \frac{\partial^2 \ln \rho}{\partial q^2} - \frac{p(q; t)^2}{\hbar^2} \right) \right],$$

and thus

$$\lim_{\delta q \rightarrow 0} \frac{\partial^2}{\partial (\delta q)^2} \ln Z(q, \delta q; t) = \frac{1}{4} \frac{\partial^2 \ln \rho(q; t)}{\partial q^2},$$

which implies equation (10), as we were willing to show.

Another way of comparing the two derivations is to substitute (15) into the equation satisfied by the characteristic function and take the real and imaginary parts to find equations (5) and (6).

These results show that the two derivations are mathematically equivalent, and their comparison gives us another perspective about the physical content of the second axiom of the characteristic function derivation. That axiom is rather mathematical and hides the physical content related to the imposition it makes upon the dispersions in position and momentum of some physical process *at each point of the configuration space*.

We now prove that relation (2), *with an equal sign for each point of the configuration space*, mathematically gives Heisenberg's dispersion relations, if one integrates it with respect to  $q$  (see, for example, [8]).

Indeed, if we begin with

$$\langle \delta p(q; t)^2 \rangle \langle \delta q(q; t)^2 \rangle = \frac{\hbar^2}{4},$$

and use

$$\langle \delta p(q; t)^2 \rangle = -\frac{\hbar^2}{4} \frac{\partial^2 \ln \rho(x, t)}{\partial x^2},$$

then

$$\overline{\Delta p^2} \cdot \overline{\Delta x^2} = -\frac{\hbar^2}{4} \int \rho(x, t) \frac{\partial^2 \ln \rho(x, t)}{\partial x^2} dx \int (x - \bar{x})^2 \rho(x, t) dx,$$

with  $\overline{\Delta p^2}$  and  $\overline{\Delta x^2}$  as implied. If we rewrite this last expression as

$$\overline{\Delta p^2} \cdot \overline{\Delta x^2} = -\frac{\hbar^2}{4} \int \left( \sqrt{\rho(x, t)} \frac{\partial \ln \rho(x, t)}{\partial x} \right)^2 dx \cdot \int \left[ \sqrt{\rho(x, t)} (x - \bar{x}) \right]^2 dx,$$

and apply the Schwartz inequality, we get

$$\overline{\Delta p^2} \cdot \overline{\Delta x^2} \geq -\frac{\hbar^2}{4} \left( \int \rho(x, t) (x - \bar{x}) \frac{\partial \ln \rho(x, t)}{\partial x} dx \right)^2,$$

and thus (after a simplification and an integration by parts)

$$\overline{\Delta p^2} \cdot \overline{\Delta x^2} \geq \frac{\hbar^2}{4}.$$

We note that one may consider the characteristic function  $Z(q, \delta q; t)$  as a momentum partition function, in the same mathematical sense that the function  $Z_e = \sum_r e^{-\beta E_r}$  of usual statistical mechanics is an energy partition function. Indeed, we may establish the close formal analogy between these two functions for the derivation of useful statistical quantities. This comparison is presented in Table 1.

The results shown in Table 1 address an old intuition first presented by Callen (see [9], pp. 458), who argued, in the realm of thermodynamics, that we should write the thermodynamic characteristic function  $Z_e$  in its most general form as

$$f_i = \frac{1}{Z} \exp \left( -\beta E_i - \vec{\lambda}_p \cdot \vec{P}_i - \vec{\lambda}_J \cdot \vec{J}_i \right),$$

where the Lagrange parameters  $(\beta, \vec{\lambda}_p, \vec{\lambda}_J)$  play the same role in the generalized theory as the parameter  $\beta$  plays in the usual formalism, and  $\vec{P}$  and  $\vec{J}$  are the linear and angular momenta, respectively.

**Table 1:** Comparison between the energy partition function and the momentum partition function as defined in the present work.

Energy Partition Function	Momentum Partition Function
$Z_e = \sum_r e^{-\beta E_r}$	$Z = \int F(q, p; t) e^{\frac{i}{\hbar} p \delta q} dp$
$\langle E \rangle = -\frac{\partial \ln Z_e}{\partial \beta}$	$\langle p \rangle = \lim_{\delta q \rightarrow 0} -i\hbar \frac{\partial \ln Z}{\partial (\delta q)}$
$\langle E^2 \rangle = \frac{1}{Z_e} \frac{\partial^2 Z_e}{\partial \beta^2}$	$\langle p^2 \rangle = \lim_{\delta q \rightarrow 0} -\frac{\hbar^2}{Z} \frac{\partial^2 Z}{\partial (\delta q)^2}$
$\langle \Delta E^2 \rangle = \frac{\partial^2 \ln Z_e}{\partial \beta^2}$	$\langle \delta p^2 \rangle = \lim_{\delta q \rightarrow 0} -\hbar^2 \frac{\partial^2 \ln Z}{\partial (\delta q)^2}$

Callen thus concludes:

“In accepting the existence of a conserved macroscopic energy function as the first postulate of thermodynamics, we anchor that postulate directly in Noether's theorem and in the time-translation symmetry of the physical laws.

An astute reader will perhaps turn the symmetry argument around. There are seven ‘first integrals of the motion’ (as the conserved quantities are known in mechanics). These seven conserved quantities are the energy, the three components of the linear momentum and the three components of the angular momentum; and they follow in parallel fashion from the translation in ‘space-time’ and from rotation. Why, then, does energy appear to play a unique role in thermostatics? Should not momentum and angular momentum play parallel roles with the energy?

In fact, the energy is not unique in thermodynamics. The linear momentum and angular momentum play precisely parallel roles. The asymmetry in our account of thermostatics is a purely conventional one that obscures the true nature of the subject.

We have followed the standard convention of restricting attention to systems that are macroscopically stationary, in which case the momentum and angular momentum are arbitrarily required to be zero and do not appear in the analysis. But astrophysicists, who apply thermostatics to rotating galaxies, are quite familiar with a more complete form of thermostatics. In that formulation the energy, the linear momentum, and the angular momentum play fully analogous roles.(...)

The proper ‘first law of thermodynamics’, (...) is the symmetry laws of physics under space-time translation and rotation, and the consequent existence of conserved energy, momentum, and angular momentum functions.” (see [9], pp. 461-462)

We note that we could have defined the characteristic function with the energy term included (multiplied by  $\delta t$ , and this is exactly what appeared when we made the connections with Feynman's formalism); the inclusion of this term would not change our derivations. Moreover, the complete ‘momentum term’, that could be written as  $\vec{\lambda}_p \cdot \vec{P}_i + \vec{\lambda}_J \cdot \vec{J}_i$  is just our term  $\vec{p} \cdot \delta \vec{q}$ , where  $\delta \vec{q}$  plays the role of the parameters  $\vec{\lambda}_p$  and  $\vec{\lambda}_J$ , if we remember that  $\vec{p}$  already includes angular momentum (as should had become clear when we approached the problem of quantization in generalized coordinates in paper I).

## 4. The Phase-Space Probability Density Function

The previous developments have very important consequences for our representation of the problem upon phase space. The equivalence between the two approaches shows us that we must identify  $\rho(q + \delta q; t)$  with  $Z(q, \delta q; t)$ , since they are exactly equal up to second order in  $\delta q$ . Then we may use (9) to invert the Fourier transform to find

$$F(q, p; t) = \frac{\rho(q; t)}{\sqrt{2\pi v(q; t)}} \exp \left\{ -\frac{[p - p(q, t)]^2}{2v(q; t)} \right\}, \quad (18)$$

where we already used

$$p(q; t) = -i\hbar \lim_{\delta q \rightarrow 0} \frac{\partial \ln Z(q, \delta q; t)}{\partial (\delta q)},$$

and we put the variance density in  $p$  as

$$v(q; t) = -\frac{\hbar^2}{4} \frac{\partial^2 \ln \rho(q; t)}{\partial q^2}.$$

Function  $v(q; t)$  (the variance on  $p$ ) will be generally positive definite. If we note that  $v(q; t) = \langle \delta p(q; t)^2 \rangle$ , expression (18) tells us that the phase space probability distribution function for any phenomenon of Quantum Mechanics is given, *at each point of the configuration space*, as a Gaussian function with average momentum given by  $p(q; t)$  and statistical variance given by  $v(q; t)$ . We have already pointed out in paper I that a Gaussian characteristic function is related to a Gaussian probability density function (for each point of the configuration space, something obviously connected to the Central Limit Theorem).

## 5. Connections with Bohm's Approach

The path taken by our derivations leaves no room for any sort of ambiguity in the calculation of average values using the probability density function  $F_n(q, p; t)$  – we are already assuming that the problem at hand is represented by some set of quantum numbers  $n$ , since we know that the Schrödinger equation will imply in the quantization of the spectrum –; given some function  $g(q, p)$ , its average value with respect to the quantum state labeled by  $n$  is calculated simply as

$$\langle g(q, p) \rangle_{n, qp}(t) = \int \int g(q, p) F_n(q, p; t) dq dp, \quad (19)$$

while its average value with respect only to the momenta (and thus defined upon configuration space) is given by

$$\langle g(q, p) \rangle_n(q; t) = \int g(q, p) F_n(q, p; t) dp.$$

Note that we have used an index in the phase space probability density function. This is just to make it

explicit that we must have one phase space probability density function, as given in (18), for each quantum mechanical state.

Thus, since we know that the expression for  $F_n$  is given by (18), we can readily calculate the expression for any function  $g(q, p)$  defined upon phase space. In particular, we may calculate these results for the energy.

The average energy density (upon configuration space) is given by

$$\langle H(q, p) \rangle_n = \int H(q, p) F_n(q, p; t) dp = h_n(q; t) \rho_n(q; t),$$

where  $H(q, p)$  is the classical Hamiltonian and  $h_n(q; t)$  is a Hamiltonian density. Now, writing

$$H(q, p) = \frac{p^2}{2m} + V(q),$$

and using (18), it is very easy to show that

$$h_n(q; t) = \frac{p_n(q; t)^2}{2m} + V(q) - \frac{\hbar^2}{8m} \frac{\partial^2 \ln \rho_n(q; t)}{\partial q^2};$$

the average energy  $e_n = \langle H(q, p) \rangle_{n, qp}$  is given by

$$e_n = \int \rho_n(q; t) \times \left( \frac{p_n(q; t)^2}{2m} + V(q) - \frac{\hbar^2}{8m} \frac{\partial^2 \ln \rho_n(q; t)}{\partial q^2} \right) dq, \tag{20}$$

where we are assuming that  $\rho_n(q; t)$  is normalized.

However, we have already shown that we must have (compare with [10])

$$\frac{\partial S_n}{\partial t} + \frac{1}{2m} \left( \frac{\partial S_n}{\partial q} \right)^2 + V(q) - \frac{\hbar^2}{2m R_n(q; t)} \frac{\partial^2 R_n}{\partial q^2} = 0,$$

and, if we have,

$$\psi_n(q; t) = R_n(q; t) \exp\left(\frac{i}{\hbar} S_n(q; t)\right),$$

such that

$$S_n(q; t) = -E_n t + f_n(q),$$

(where  $E_n$  is the energy calculated using the Schrödinger equation), as is usual. We find that (we also write  $p_n(q; t)$  for  $\partial S_n(q; t)/\partial q$ )

$$E_n = \frac{p_n(q; t)^2}{2m} + V(q) - \frac{\hbar^2}{2m R_n(q; t)} \frac{\partial^2 R_n}{\partial q^2},$$

and thus, giving the normalization of  $\rho_n(q; t)$ , we must have

$$E_n = \int \rho_n(q; t) \times \left[ \frac{p_n(q; t)^2}{2m} + V(q) - \frac{\hbar^2}{2m R_n(q; t)} \frac{\partial^2 R_n}{\partial q^2} \right] dq, \tag{21}$$

since  $E_n$  is a constant. Now, we must compare  $E_n$  with  $e_n$ . We may differentiate the last term in (20) and use the fact that  $\rho_n(q; t)$  is a probability density to find, using  $\rho_n(q; t) = R_n(q; t)^2$ ,

$$E_n = \int \left\{ \rho_n(q; t) \left\{ \frac{p_n(q; t)^2}{2m} + V(q) + \frac{\hbar^2}{2m} \left( \frac{\partial R_n(q; t)}{\partial q} \right)^2 \right\} \right\} dq$$

and integration by parts in the last term gives directly (21). Thus,  $E_n = e_n$  and our criterion to calculate the energy is shown to be sound.

It is now better to take a look at some examples to see, in less abstract ways, how the formalism works.

## 6. Examples

### 6.1. The one-dimensional harmonic oscillator example

The harmonic oscillator problem has solutions given by

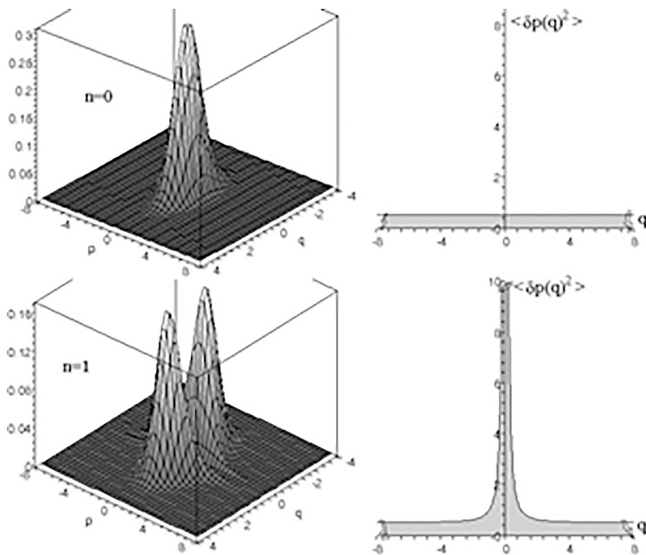
$$\psi_n(q) = \left( \frac{\beta}{\pi 2^{2n} n!} \right)^{1/4} \exp\left(-\frac{\beta q^2}{2}\right) H_n(\sqrt{\beta} q), \tag{22}$$

where  $\beta = m\omega/\hbar$ , and  $H_n(\sqrt{\beta} q)$  are the Hermite polynomials. In Table 2 we present the probability density function  $F_n(q, p; t)$  for various values of  $n$ . The distribution functions defined upon phase space quickly get very complicated, but the process to find them is immediate and any algebraic computer program can do the job (we present such a program in the appendix). The dispersions  $\Delta p_n$  and  $\Delta q_n$  and the energy  $E_n$  can also be calculated using the functions presented in Table 2 and the results are the usual ones (again, algebraic computation was used throughout).

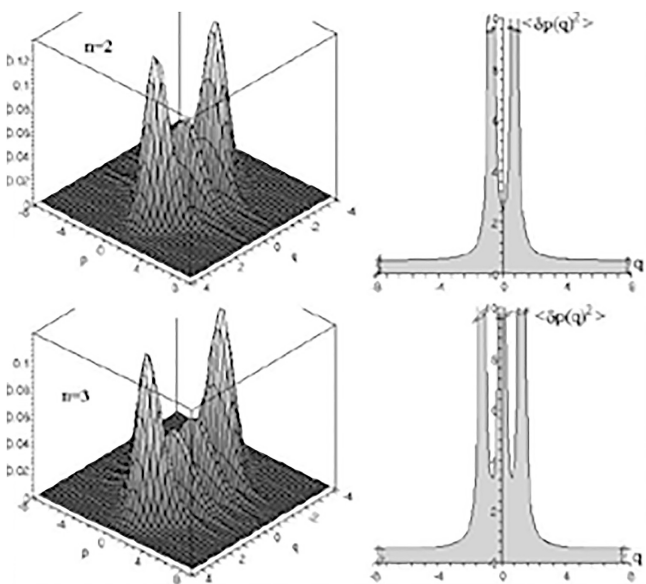
We can plot these phase space probability distributions for each value of the quantum number  $n$ . The results are shown in Figure 2, together with the profile of the average fluctuations  $\langle \delta p(q)^2 \rangle$ .

**Table 2:** Phase space probability density functions for various values of the quantum number  $n$  for the harmonic oscillator problem.

$n$	$F_n(q, p)$	$E_n$
0	$\frac{1}{\pi} e^{-\beta q^2 - \frac{p^2}{\hbar^2 \beta}}$	$\frac{1}{2}$
1	$\frac{2 \sqrt{\beta} q ^3}{\pi \hbar \sqrt{\beta q^2 + 1}} e^{-\beta q^2 - \frac{p^2 q^2}{\hbar^2 (\beta q^2 + 1)}}$	$\frac{3}{2}$
2	$\frac{ 2\beta q^2 - 1 ^3}{2\pi \hbar \sqrt{2\beta^2 q^4 + 4\beta q^2 + 5}} e^{-\beta q^2 - \frac{p^2 (2\beta q^2 - 1)^2}{\hbar^2 \beta (2\beta^2 q^4 + 4\beta q^2 + 5)}}$	$\frac{5}{2}$
3	$\frac{ \sqrt{\beta} q (2\beta q^2 - 3) ^3}{3\pi \hbar \sqrt{4\beta^3 q^6 + 9\beta^2 q^2 + 9}} e^{-\beta q^2 - \frac{p^2 q^2 (2\beta q^2 - 3)^2}{\hbar^2 (4\beta^3 q^6 + 9\beta^2 q^2 + 9)}}$	$\frac{7}{2}$



**Figure 2:** Left column: The phase space probability density functions for \$n=0\$ and \$n=1\$. Right column: the average fluctuation profiles defined upon configuration space.



**Figure 3:** Left column: The phase space probability density functions for \$n=2\$ and \$n=3\$. Right column: the average fluctuation profiles defined upon configuration space.

The fluctuation profiles may be compared to the contours of the probability density functions to make a first tentative interpretation of the results – an interpretation that we will keep improving in future papers. Let us consider the state \$n = 1\$ of the quantum harmonic oscillator. The function \$F\_1(q, p; t)\$ is given in Table 2 and the momentum fluctuation profiles are given (for \$n = 0, 1, 2, 3\$) in Figure 2 and Figure 3 (compare with the results in [11]).

The Schrödinger equation can be written in the format

$$\frac{\partial p_1(q; t)}{\partial t} = -\frac{\partial}{\partial q} \left( \frac{p_1(q; t)^2}{2m} + V(q) - \frac{\hbar^2}{8m} \frac{\partial^2 \ln \rho_1(q; t)}{\partial q^2} \right),$$

where we used (17). This equation can be rewritten as

$$\frac{\partial p_1(q; t)}{\partial t} + \frac{p_1(q; t)}{m} \frac{\partial p_1(q; t)}{\partial q} = -\frac{\partial V(q)}{\partial q} - \frac{\partial Q_1(q)}{\partial q},$$

where

$$Q(q) = -\frac{\hbar^2}{8m} \frac{\partial^2 \ln \rho_1(q; t)}{\partial q^2},$$

and it can be *metaphorically* identified with the Hamilton equation

$$\frac{dp_1}{dt} = -\frac{\partial V(q)}{\partial q} - \frac{\partial Q_1(q)}{\partial q}, \tag{23}$$

as David Bohm did in his seminal papers [10]. In the present approach, however, the function \$Q\_1(q)\$ cannot be associated with a true potential, but reflects only the momentum fluctuations<sup>2</sup>. This shows that Bohm's approach cannot be assumed as a non-statistical deterministic theory (analogous to Newtonian Mechanics, but with an extra potential function), as is amply assumed. Indeed, its main variable \$p\$ is, in fact, a statistical *function*. Moreover, equation (23) is *not* a true Hamiltonian equation, since, in the present approach, \$p\$ is, in fact, \$p(q; t)\$, an explicit function of \$q\$, and not an independent variable, as required for a true Hamilton-Jacobi theory. This, in turn, easily explains why, for stationary and symmetrical states in general, one gets \$p(q; t) = 0\$, something hard to explain using Bohm's interpretation of the formalism.

Having said this, we can turn our attention to a simple example, using equation (23) to write it, for the first excited state of the Harmonic Oscillator, by substituting the expression for the derivatives there shown. We then find that our "Hamiltonian" for equation (23) is given by (we also write the potential of the harmonic oscillator)

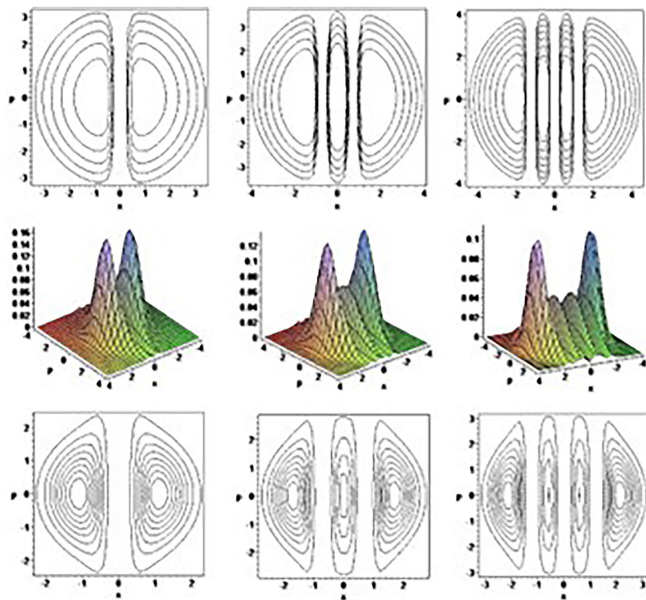
$$H(q, p_1) = \frac{p_1^2}{2m} + \frac{1}{2}m\omega^2 q^2 + \frac{\hbar^2}{2m} \left( \frac{1+q^2}{q^2} \right),$$

$$Q(q) = \frac{\hbar^2}{2m} \left( \frac{1+q^2}{q^2} \right),$$

We can draw the constant energy trajectories for the previous Hamiltonian (see the appendix) and they are shown in Figure 4. We also show in Figure 4 the contours of the probability density function \$F\_1(q, p; t)\$. These two sets of contours present a striking resemblance to each other showing that the constant probability curves of the function \$F\_1(q, p; t)\$ are close to the constant energy ones, although not exactly the same.

<sup>2</sup> This may induce us to try to find a Langevin equation for Quantum Mechanics, something we will do in a future paper of this series.





**Figure 4:** Contours of the Hamiltonian and of the probability density function for the levels  $n=1, 2$  and  $3$  of the harmonic oscillator problem. For the Hamiltonian, each contour represents a constant energy shell, while, for the probability density function, each contour represents a constant probability density.

Most important, these two sets of contours give us a clue of what is going on in the detailed microscopic level. Indeed, we may see that the term given by  $Q_1(q)$  has a divergence at the origin; thus if the particle (of whose position  $q$  is a label – remember: Feynman’s path integrals allows us to use these notions) is on a constant energy contour, whenever it comes close to the origin, there appears a very strong force which will be responsible for drastically altering the value of the particle’s momentum. This explains the strong modifications in value that the momenta suffer at points close to the origin, even if the coordinate  $q$  is not substantially altered. The corpuscle then is strongly thrown away from the origin. This can be seen by the fluctuation profile for the fluctuation in the momentum, shown in Figure 3, by the tangents lines of the contours at regions close to the origin. At great distances from the origin, the term given by  $Q_1(q)$  becomes almost constant and does not produce any appreciable force; thus, the system behaves exactly as a usual harmonic oscillator and the contours approach the form of a circle (or an ellipse, in general). The contours of the probability density function  $F_1(q, p; t)$  just reproduce this pattern: since the corpuscle has a tendency to be pushed from the origin, the probability of finding it there is very low (zero, indeed, since there  $Q_1(q)$  goes to infinity). The exact same analysis can be made for all excited states.

### 6.2. The Hydrogen atom example

Let us now take the Hydrogen atom problem, for which the normalized probability density function is given by

(we put  $m = \hbar = a = e = 1$  and  $\vec{x} = (r, \theta, \phi)$ )

$$\rho_n(\vec{x}) = R_{n\ell}(r)^2 |Y_{\ell m}(\theta, \phi)|^2, \tag{24}$$

where

$$R_{n\ell}(r) = -\left(\frac{2}{n}\right)^{3/2} e^{-r/n} \left(\frac{2r}{n}\right)^\ell L_{n+\ell}^{2\ell+1}\left(\frac{2r}{n}\right) \tag{25}$$

with  $L_k^s(x)$  the associated Laguerre functions and

$$Y_{\ell m}(\theta, \phi) = \left[\frac{2\ell+1}{4\pi} \frac{(\ell+|m|)!}{(\ell-|m|)!}\right]^{1/2} P_\ell^m(\theta) e^{im\phi} \tag{26}$$

are the usual spherical harmonics with  $P_\ell^m(\theta)$  the associated Legendre functions. We thus have

$$p_\phi(\vec{r}; t) = \nabla S(\vec{x}; t) = \frac{m}{r \sin \theta} \hat{\phi}, \tag{27}$$

that we got from  $S(\vec{x}; t) = E + m\phi$ .

In Table 3 we have listed quantum numbers for some states of the hydrogen atom together with their momentum fluctuations, in the first and second columns, respectively. The energy values obtained by explicit calculation of the integral (19) with  $g(q, p)$  equal to the Hamiltonian function are given in the third column. The results are exactly those found for the Hydrogen atom (algebraic computation used throughout, see Appendix 2).

In spherical coordinates, the phase space probability density functions, for a three dimensional problem, are written in the general format

$$F(\vec{r}, \vec{p}) = \frac{\rho(\vec{r})}{[2\pi m k_B T(q; t)]^{3/2}} \exp\left\{-\frac{[\vec{p} - \overline{p(q; t)}]^2}{2m k_B T(q; t)}\right\}, \tag{28}$$

which represents a Maxwellian function, where  $\overline{p(q; t)}$  is an average momentum, and  $T(q; t)$  is the local temperature. Since we have (27), we get

$$[\vec{p} - \nabla S(\vec{r})]^2 = p_r^2 + \frac{p_\theta^2}{r^2} + \frac{(p_\phi - m)^2}{r^2 \sin^2 \theta}.$$

We also have

$$\frac{3}{2} k_B T(q; t) = \langle \delta \vec{p}(\vec{r})^2 \rangle = -\frac{\hbar^2}{4} \nabla^2 \ln \rho(\vec{r}), \tag{29}$$

**Table 3:** Momentum fluctuations and energies for some states of the hydrogen atom problem given by the quantum numbers in the first column ( $\xi = \cos \theta$ ).

$(n, \ell, m)$	Momentum Fluctuations	E
(1,0,0)	$\frac{1}{r}$	$-\frac{1}{2}$
(2,0,0)	$\frac{1}{2} \frac{(8-5r+r^2)}{r(r-2)^2}$	$-\frac{1}{8}$
(2,1,0)	$\frac{1}{2} \frac{r\xi^2+1}{r^2\xi^2}$	$-\frac{1}{8}$
(2, 1, $\pm 1$ )	$\frac{1}{2r}$	$-\frac{1}{8}$
(3,0,0)	$\frac{1}{3} \frac{2187-1944r+648r^2-84r^3+4r^4}{r(27-18r+2r^2)^2}$	$-\frac{1}{18}$
(3,1,0)	$\frac{1}{6} \frac{108r\xi^2-27r^2\xi^2+2r^3\xi^2+108-36r+3r^2}{r^2(r-6)^2\xi^2}$	$-\frac{1}{18}$
(3,1, $\pm 1$ )	$\frac{1}{6} \frac{(-27r+108+2r^2)}{r(r-6)^2}$	$-\frac{1}{18}$

**Table 4:** Phase space probability density functions for some levels of the hydrogen atom ( $\xi = \cos \theta$ ) and the functions are not normalized.

$(n, \ell, m)$	$F(r, \theta, \phi, p_r, p_\theta, p_\phi; t)$
(1,0,0)	$r^{3/2} e^{-2r} e^{-\frac{3}{2} \left[ p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2 \theta} \right]} r$
(2,0,0)	$\frac{r^{3/2}  r-2 ^5}{(8-5r+r^2)^{3/2}} e^{-r} e^{-3 \left[ p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2 \theta} \right]} \frac{r(r-2)^2}{8-5r+r^2}$
(2,1,0)	$\frac{ r\xi ^5 e^{-r} e^{-3 \left[ p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2 \theta} \right]} (\xi^2 r + 1)^{3/2}}{\xi^2 r + 1}$
(2,1,1)	$r^{7/2} \sin^2 \theta e^{-r} e^{-3 \left[ p_r^2 + \frac{p_\theta^2}{r^2} + \frac{(p_\phi - 1)^2}{r^2 \sin^2 \theta} \right]} r$

since we are in three dimensions. Thus, we end with

$$F(\vec{r}, \vec{p}) = \frac{\rho(\vec{r})}{[2\pi \langle \delta \vec{p}(\vec{r})^2 \rangle / 3]^{3/2}} \exp \left\{ -\frac{3 [\vec{p} - m]^2}{2 \langle \delta \vec{p}(\vec{r})^2 \rangle} \right\}. \quad (30)$$

In Table 4, we write the probability density functions in phase space for some levels of the hydrogen atom.

### 7. Zeroes of the Integrated Liouville Equation

In paper I, we *postulated* in axiom 1 that

$$\int \exp \left( \frac{i}{\hbar} p \delta q \right) \frac{dF(q, p; t)}{dt} dp = 0, \quad (31)$$

but the function  $F(q, p; t)$  was not available. Now, with this function at hand, we may show that this is indeed the case, up to second order in  $\delta q$ .

Note that we *do not* assume that the function  $F$  is a solution of the Liouville equation (which would make the whole formalism of Quantum Mechanics to collapse into the Newtonian one).

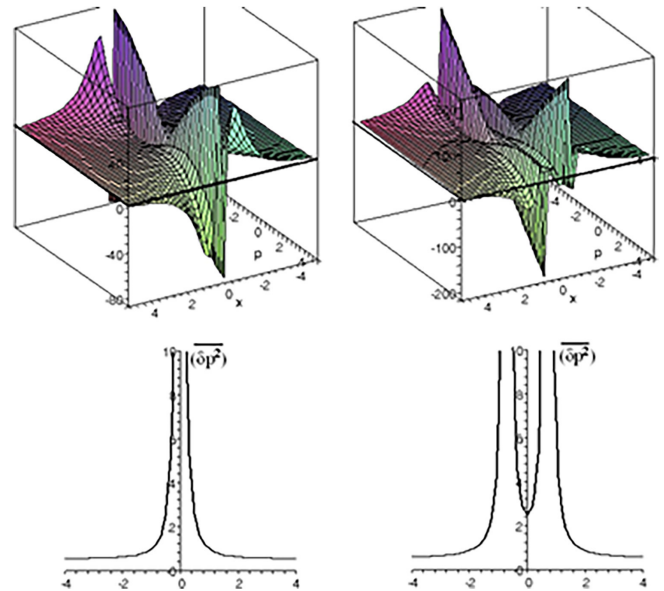
Now, with the probability density function at hand, we can, for the examples in the previous section, explicitly calculate this result. This calculation is presented in the Maple program that we make available at appendix A. We do that by showing that

$$\int_{-\infty}^{\infty} \left[ \lim_{\delta q^2 \rightarrow 0} \int_{-\infty}^{\infty} \exp \left( \frac{i}{\hbar} p \delta q \right) \frac{F_n(x, p)}{dt} dp \right] dq = 0, \quad (32)$$

for  $n = 0, 1, 2, 3, \dots$ , as expected.

Although we are not assuming that the phase space probability density function satisfies the Liouville equation, it is instructive to consider the application of the Liouville operator to the quantum phase space probability density.

Again, for the simplest case of the harmonic oscillator in the first and second excited states ( $F_1$  and  $F_2$ ), we get the results shown in Figure 5 (we divided the application of the Liouville operator by  $F_n$  to avoid the fact of



**Figure 5:** Behavior of the functions  $F_n(q, p)$  for  $n = 1$  and  $n = 2$ . The images show the strong fluctuation behavior of the phase space density near the divergence points in the momentum fluctuations, while they satisfy Liouville's equation far from the divergence points.

making the result to go to zero because of the negative Gaussian exponent). That is, in Figure 5 we plot the function

$$\frac{1}{F_n(q, p)} \frac{dF_n(q, p)}{dt} = \frac{1}{F_n(q, p)} \left( \frac{p}{m} \frac{\partial F_n}{\partial q} - q \frac{\partial F_n}{\partial p} \right), \quad (33)$$

and similar plots can be obtained for any quantum number  $n$  (see Appendix A).

In this figure it becomes apparent that the Liouville equation is, indeed, satisfied *almost* everywhere, *except* at the points where the phase-space probability density functions have divergences. At those points, the results resemble some sort of fluctuation process. This explains why the contours of the phase-space probability density function are not exactly the same as the energy contours: if they were the same, the phase-space probability density function would obey, exactly, the Liouville equation and Quantum Mechanics would collapse into Newtonian Mechanics. However, it becomes apparent that the integral in (31) does the job of averaging over these fluctuation behavior – a point to which we will return in future papers.

### 8. Entropy Maximization and Energy Minimization

Another interesting argument in favor of  $F(x, p)$  can be found in the literature connected with the Density Functional Theory (DFT). It can be easily shown that  $F(q, p)$  is the distribution function that maximizes the

local Boltzmann’s entropy

$$\mathfrak{S}(q) = -k_B \int \int F(\vec{q}, \vec{p}) \ln F(\vec{q}, \vec{p}) d\vec{q}d\vec{p} \quad (34)$$

constrained to satisfy

$$\rho(\vec{q}) = \int F(\vec{q}, \vec{p}) d\vec{p} \quad t_s(\vec{q}) = \int \frac{\vec{p}^2}{2} F(\vec{q}, \vec{p}) d\vec{p},$$

where  $t_s(\vec{q})$  is the so called Weiszäcker term in the context of Density Functional Theory (see [12], pp. 239–240). It is then possible to define notions such as local temperature, pressure etc.

Given this last result, we can show by other means that  $F(\vec{q}, \vec{p})$  is the probability density function related to the Schrödinger equation. Indeed, the *energy functional* becomes, using our previous result (20)

$$\begin{aligned} E[\rho, \nabla\rho] &= \int \int H(\vec{q}, \vec{p}) F(\vec{q}, \vec{p}) d\vec{r}d\vec{p} \\ &= \int \left\{ \left[ \frac{p(q,t)^2}{2m} + V(\vec{q}) \right] \rho(\vec{q}) + \frac{\hbar^2}{8m} \frac{|\nabla\rho|^2}{\rho} \right\} d\vec{q}, \end{aligned}$$

where we used in the last equality the fact that  $\rho(\vec{q})$  must be zero when  $\vec{q} \rightarrow \infty$ . With this functional we can make our variations [with the Lagrange multiplier  $\lambda$  introduced by the normalization of the probability density  $\rho(\vec{q})$ ] to find

$$\begin{aligned} \frac{\delta E[\rho, \nabla\rho]}{\delta\rho} &= -\frac{\hbar^2}{4m} \nabla \cdot \left( \frac{\nabla\rho}{\rho} \right) - \frac{\hbar^2}{8m} \frac{|\nabla\rho|^2}{\rho^2} + \frac{p(\vec{q}, t)^2}{2m} + V(\vec{q}) - \lambda \\ &= -\frac{\hbar^2}{4m} \left[ \frac{\nabla^2\rho}{\rho} - \frac{1}{2} \frac{|\nabla\rho|^2}{\rho^2} \right] + \frac{p(\vec{q}, t)^2}{2m} + V(\vec{q}) = \lambda, \end{aligned}$$

and when we put, as usual,  $\rho(\vec{q}, t) = R(\vec{q}, t)^2$  and  $\vec{p}(\vec{q}, t) = \nabla S(\vec{q}, t)$ , we find

$$\frac{1}{2m} |\nabla s(\vec{q}, t)|^2 + V(\vec{q}) - \frac{\hbar^2}{2mR(\vec{q}, t)} \nabla^2 R(\vec{q}, t) = \lambda.$$

This last equation is completely equivalent to (12) for stationary states for which

$$\frac{\partial S(\vec{q}, t)}{\partial t} = \lambda,$$

being  $\lambda$ , obviously, the energy of the state.

### 9. Extensions for Teaching Physics

It is worth highlighting the effort, made in this article, of the axiomatic derivation of the Schrödinger equation from Boltzmann’s entropy construct, demonstrating the connections with the positive probability distribution function – defined in phase space. Furthermore, we

sought to characterize it as the only one capable of maximizing entropy simultaneously while minimizing energy, while Bohmian Mechanics is considered and reinterpreted from the perspective developed from the mathematical results of this approach.

Based on discussions carried out in previous articles by these authors, for example in [2, 3, 13, 14], we consider that the approach and examples elaborated in this text are transposable to common teaching situations in Higher Education, such as initial Quantum Mechanics courses.

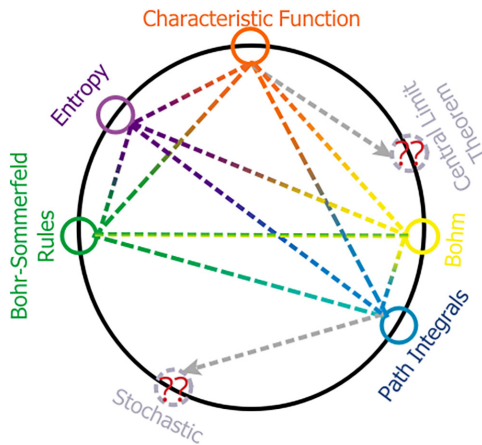
This development, in a logic of didactic transposition [1–3, 15], can favor reasoning skills, concept formation, investigation and translation for the constitution of careful, critical and creative higher order thinking. This is in line with perspectives of meaningful [16, 17] and critical [18, 19] learning, especially when we understand a capacity to disrupt the hegemonic model of presenting the Schrödinger equation as a separate postulate, often obtained from principles of symmetry, usually dedicated to describing wave-particle duality.

It would also be possible to imagine going further and treating more general systems, for example, via application to systems with speed-dependent potentials, which, in fact, we will show in a future article as an example of an extension of the approach. Thus, such modeling could, for example, dedicate itself rigorously to dissipative systems, finding a more general Schrödinger equation that takes such effects into account – something that has been attempted, in various ways, since the birth of Quantum Mechanics.

Works like this seek to provide alternatives that provide the student with entry into the field of Quantum Mechanics beyond the usual form, provided by manuals that are endlessly repeated, without bringing anything beyond a carefree formalism of questions of interpretation. Very important to highlight, they do this without foregoing the necessary formalism, which works, in fact, as an elucidator of the interpretative structures that underlie it, and they do so, specifically through the derivation model adopted, which allows the interpretation of numerous constructs and variables of Quantum Mechanics to starting from the idea that, in the derivation process, such variables that emerge from mathematical developments inherit their meaning from those placed in the axioms – something that a non-axiomatic derivation would never be able to achieve.

### 10. Final Considerations

In this paper, the second of the series on mathematical quantization procedures, we improve our knowledge of some deep aspects of Quantum Mechanics. For instance, the role played by Boltzmann’s entropy (and, thus, the extensional aspect of the theory) and some very stringent interpretational issues regarding Bohm’s approach, now based on solid formal derivation, instead of an analogy



**Figure 6:** New connections between formal results regarding quantization and the formalism of Quantum Mechanics. Bohmian Mechanics, in a new perspective, and a derivation based on Boltzmann's entropy are now part of results.

loosely established. In terms of Figure 1 we now have the situation shown in Figure 6.

We must stress two things regarding Figure 6. First, we are assuming transitivity of mathematical derivations, which should be obvious. Then, if one can connect the entropy derivation with the Characteristic Function one, and it was mathematically proved that the Characteristic Function derivation is equivalent to Feynman's Path Integral approach, there is no need to show the formal equivalence between Feynman's approach and the Entropy one. This is important. Such a relation would be very difficult to formally establish, showing, again, the importance of having different quantization methods as a means to better understand the theory. This kind of approach may help teachers of undergraduate courses to introduce important discussions about the interpretation of Quantum Mechanics. We kept the formalism at this level of presentation and make it accessible algebraic computation programs to present algebraically more involved results.

The second important thing to mention is that, we still have not accomplished the formal derivation of the two connections of the present approach with (a) the Central Limit Theorem and (b) some possible stochastic behavior, of which Figure 6 is but mere *suggestive*, although we have given one more step towards that. We thus *refrain* from making wild interpretations using these constructs and keep ourselves within the stringent epistemological decision of saying something about the interpretation of Quantum Mechanics only after having it proved in the mathematical formalism. This will help us not assuming, *a priori* and *ad hoc*, the existence of many worlds, "wholenesses" (as was shown for the Bohmian approach), and other assumptions generally found in the interpretation of Quantum Mechanics.

These results will be shown to be valid in future papers.

## Acknowledgments

The National Council for Scientific and Technological Development (CNPq).

## Supplementary material

The following online material is available for this article Appendix A – Maple program to study the Harmonic Oscillator problem.

Appendix B – Maple program to study the Hydrogen Atom problem.

## References

- [1] L.S.F. Olavo and M. Ferreira, Rev. Bras. Ens. Fís. **46**, e20240183 (2024).
- [2] L.S.F. Olavo and M. Ferreira, Rev. Bras. Ens. Fís. **43**, e20200508 (2021).
- [3] L.S.F. Olavo, M. Ferreira and R.G.G. Amorim, Rev. Bras. Ens. Fís. **44**, e20220109 (2022).
- [4] L.S.F. Olavo, Physica A: Statistical Mechanics and its Applications **271**, 260 (1999).
- [5] R. Liboff, *Kinetic Theory* (Prentice-Hall, New Jersey, 1990).
- [6] M. Born, *Natural Philosophy of Cause and Chance* (Oxford University Press, Oxford, 1949).
- [7] F. Reif, *Fundamentals of Statistical and Thermal Physics* (McGraw-Hill, Singapore, 1965).
- [8] T. Takabayasi, Prog. Theoret. Phys. **11**, 341 (1954).
- [9] H.B. Callen, *Thermodynamics: an introduction to thermostatistics* (John Wiley & Sons, New York, 1985).
- [10] D. Bohm, Phys. Rev. **85**, 166 (1952).
- [11] M. Hillery, R.F. O'Connell, M.O. Scully and E.P. Wigner, Phys. Rep. **106**, 121 (1984).
- [12] R.G. Parr and W. Yang, *Density-functional theory of atoms and molecules* (Oxford University Press, New York, 1986).
- [13] L.S.F. Olavo and M. Ferreira, Rev. Bras. Ens. Fís. **45**, e20230231 (2023).
- [14] L.S.F. Olavo, *Quantum Mechanics: Principles, New Perspectives, Extensions, and Interpretation* (Nova Publishers, New York, 2016).
- [15] M. Ferreira, L.S.F. Olavo, M.C. Batista, A.A. Filho, A. Strapasson and A.E. Santana, Rev. Bras. Ens. Fís. **45**, e20230254 (2023).
- [16] M. Ferreira, L.S.F. Olavo, M.A. Moreira, G.B. Franz, K.O. Portugal and D.X.P. Nogueira, Rev. Bras. Ens. Fís. **42**, e20200057 (2020).
- [17] M. Ferreira, R.V.L. Couto, L.S.F. Olavo, L. Paulucci and F.F. Monteiro, Rev. Bras. Ens. Fís. **43**, e20210157 (2021).
- [18] A. Strapasson, M. Ferreira, D. Cruz-Cano, J. Woods, M.P.N.M. Soares and L.S.F. Olavo, International Journal of Educational Technology in Higher Education **19**, 1 (2022).
- [19] M. Ferreira, L.S.F. Olavo, A.B.S. Nascimento and A.B. Strapasson, Humanities & Social Sciences Communications **10**, 768 (2023).