

Complementarity in Quantum Mechanics and Classical Statistical Mechanics

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1. Introduction

Roughly speaking, *complementarity* can be understood as the coexistence of multiple properties in the behavior of an object that seem to be *contradictory*. Although it is possible to switch among different descriptions of these properties, in principle, it is impossible to view them, at the same time, despite their simultaneous coexistence. Therefore, the consideration of all these contradictory properties is absolutely necessary to provide a *complete characterization* of the object. In physics, complementarity represents a basic principle of *quantum theory* proposed by Niels Bohr (1; 2), which is closely identified with the *Copenhagen interpretation*. This notion refers to effects such as the so-called *wave-particle duality*. In an analogous perspective as the finite character of the speed of light c implies the impossibility of a sharp separation between the notions of *space* and *time*, the finite character of the *quantum of action* \hbar implies the impossibility of a sharp separation between the behavior of a quantum system and its interaction with the measuring instruments.

In the early days of quantum mechanics, Bohr understood that *complementarity* cannot be a unique feature of quantum theories (3; 4). In fact, he suggested that the thermodynamical quantities of temperature T and energy E should be complementary in the same way as position q and momentum p in quantum mechanics. According to thermodynamics, the energy E and the temperature T can be simultaneously defined for a thermodynamic system in equilibrium. However, a complete and different viewpoint for the energy-temperature relationship is provided in the framework of classical statistical mechanics (5). Inspired on Gibbs canonical ensemble, Bohr claimed that a *definite temperature* T can only be attributed to the system if it is submerged into a *heat bath*¹, in which case fluctuations of energy E are unavoidable. Conversely, a definite energy E can only be assigned when the system is put into *energetic isolation*, thus excluding the simultaneous determination of its temperature T .

At first glance, the above reasonings are remarkably analogous to the Bohr's arguments that support the complementary character between the coordinates \mathbf{q} and momentum \mathbf{p} . Dimensional analysis suggests the relevance of the following uncertainty relation (6):

$$\Delta E \Delta(1/T) \geq k_B, \quad (1)$$

where k_B is the Boltzmann's constant, which can play in statistical mechanics the counterpart role of the Planck's constant \hbar in quantum mechanics. Recently (7–9), we have shown that

¹ A heat bath is a huge extensive system driven by short-range forces, whose heat capacity C is so large that it can be practically regarded infinite, e.g.: the natural environment.

Bohr's arguments about the complementary character between energy and temperature, as well as the inequality of Eq.(1), are not strictly correct. However, the essential idea of Bohr is relevant enough: uncertainty relations can be present in any physical theory with a statistical formulation. In fact, *the notion of complementarity is intrinsically associated with the statistical nature of a given physical theory.*

The main interest of this chapter is to present some general arguments that support the statistical relevance of complementarity, which is illustrated in the case of classical statistical mechanics. Our discussion does not only demonstrate the existence of complementary relations involving thermodynamic variables (7–9), but also the existence of a remarkable analogy between the conceptual features of quantum mechanics and classical statistical mechanics.

This chapter is organized as follows. For comparison purposes, we shall start this discussion presenting in section 2 a general overview about the orthodox interpretation of complementarity of quantum mechanics. In section 3, we analyze some relevant *uncertainty-like inequalities* in two approaches of classical probability theory: *fluctuation theory* (5) and *Fisher's inference theory* (10; 11). These results will be applied in section 4 for the analysis of complementary relations in classical statistical mechanics. Finally, some concluding remarks and open problems are commented in section 5.

2. Complementarity in quantum mechanics: A general overview

2.1 Complementary descriptions and complementary quantities

Quantum mechanics is a theory hallmarked by the *complementarity* between two descriptions that are unified in classical physics (1; 2):

1. *Space-time description*: the parametrization in terms of coordinates \mathbf{q} and time t ;
2. *Dynamical description*: This description is based on the applicability of the *dynamical conservation laws*, where enter dynamical quantities as the energy and the momentum.

The breakdown of classical notions as the concept of *point particle trajectory* [$\mathbf{q}(t), \mathbf{p}(t)$] was clearly evidenced in Davisson and Germer experiment and other similar experiences (12). To illustrate that electrons and other microparticles undergo *interference* and *diffraction* phenomena like the ordinary waves, in Fig.1 a schematic representation of electron interference by double-slits apparatus is shown (13). According to this experience, the *measurement results* can only be described using classical notions compatible with its corpuscular representations, that is, in terms of the *space-time description*, e.g.: a spot in a photographic plate, a recoil of some movable part of the instrument, etc. Moreover, these experimental results are generally *unpredictable*, that is, they show an intrinsic *statistical nature* that is governed by the wave behavior dynamics. According to these experiments, there is no a sharp separation between the *undulatory-statistical* behavior of microparticles and the space-time description associated with the interaction with the measuring instruments.

Besides the existence of complementary descriptions, it is possible to talk about the notion of *complementary quantities*. Position \mathbf{q} and momentum \mathbf{p} , as well as time t and energy E , are relevant examples complementary quantities. Any experimental setup aimed to study the exchange of energy E and momentum \mathbf{p} between microparticles must involve a measure in a finite region of the space-time for the definition of wave frequency ω and vector \mathbf{k} entering in *de Broglie's relations* (14):

$$E = \hbar\omega \text{ and } \mathbf{p} = \hbar\mathbf{k}. \quad (2)$$

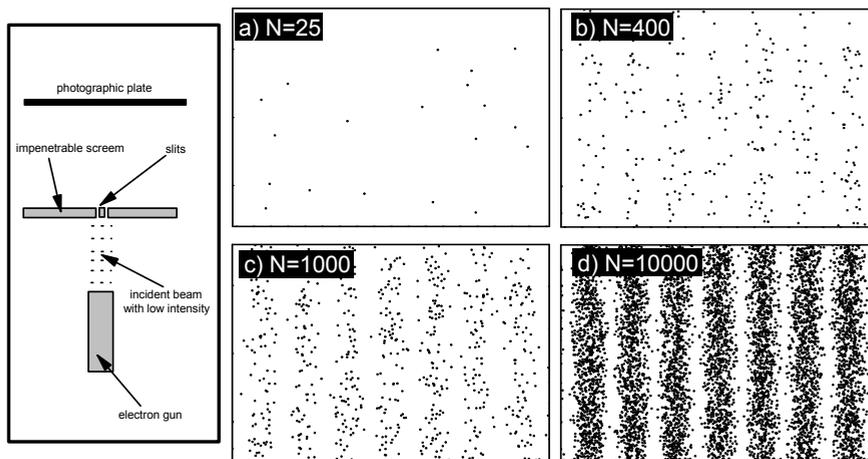


Fig. 1. Schematic representation of electron interference by double-slit apparatus using an incident beam with low intensity. Sending electrons through a double-slit apparatus one at a time results in single *spot* appearing on the photographic plate. However, an interference pattern progressively emerges when the number N of electrons impacted on the plate is increased. The emergence of an interference pattern suggested that each electron was *interfering with itself*, and therefore in some sense the electron had to be going through both slits at once. Clearly, this interpretation contradicts the classical notion of particles trajectory.

Conversely, any attempt of locating the collision between microparticles in the space-time more accurately would exclude a precise determination in regards the balance of momentum \mathbf{p} and energy E . Quantitatively, such complementarity is characterized in terms of *uncertainty relations* (2):

$$\Delta q \Delta p \geq \hbar \text{ and } \Delta t \Delta E \geq \hbar, \quad (3)$$

which are associated with the known *Heisenberg's uncertainty principle*: if one tries to describe the dynamical state of a microparticle by methods of classical mechanics, then precision of such description is limited. In fact, the classical state of microparticle turns out to be badly defined. While the coordinate-momentum uncertainty forbids the classical notion of trajectory, the energy-time uncertainty accounts for that a state, existing for a short time Δt , cannot have a definite energy E .

2.2 Principles of quantum mechanics

2.2.1 The wave function Ψ and its physical relevance

Dynamical description of a quantum system is performed in terms of the so-called the *wave function* Ψ (12). For example, such as the frequency ω and wave vector \mathbf{k} observed in electron diffraction experiments are related to dynamical variables as energy E and momentum \mathbf{p} in terms of de Broglie's relations (2). Accordingly, the wave function $\Psi(\mathbf{q}, t)$ associated with a *free microparticle* (as the electrons in a beam with very low intensity) behaves as follows:

$$\Psi(\mathbf{q}, t) = C \exp[-i(Et - \mathbf{p} \cdot \mathbf{q})/\hbar]. \quad (4)$$

Historically, de Broglie proposed the relations (2) as a direct generalization of quantum hypothesis of light developed by Planck and Einstein for any kind of microparticles (14). The

experimental confirmation of these wave-particle duality for any kind of matter revealed the unity of material world. In fact, wave-particle duality is a property of matter as universal as the fact that any kind of matter is able to produce a gravitational interaction.

While the *state* of a system in classical mechanics is determined by the knowledge of the positions \mathbf{q} and momenta \mathbf{p} of all its constituents, the state of a system in the framework of quantum mechanics is determined by the knowledge of its wave function $\Psi(\mathbf{q}, t)$ (or its generalization $\Psi(\mathbf{q}^1, \mathbf{q}^2, \dots, \mathbf{q}^n, t)$ for a system with many constituents, notation that is omitted hereafter for the sake of simplicity). In fact, the knowledge of the wave function $\Psi(\mathbf{q}, t_0)$ in an initial instant t_0 allows the prediction of its future evolution prior to the realization of a measurement (12). The wave function $\Psi(\mathbf{q}, t)$ is a complex function whose modulus $|\Psi(\mathbf{q}, t)|^2$ describes the *probability density*, in an absolute or relative sense, to detect a microparticle at the position \mathbf{q} as a result of a *measurement* at the time t (15). Such a statistical relevance of the wave function $\Psi(\mathbf{q}, t)$ about its relation with the experimental results is the most condensed expression of complementarity of quantum phenomena.

Due to its statistical relevance, the reconstruction of the wave function $\Psi(\mathbf{q}, t)$ from a given experimental situation demands the notion of *statistical ensemble* (12). In electron diffraction experiments, each electron in the beam manifests undulatory properties in its dynamical behavior. However, the interaction of this microparticle with a measuring instrument (a classical object as a photographic plate) radically affects its initial state, e.g.: electron is forced to localize in a very narrow region (the spot). In this case, a single measuring process is useless to reveal the wave properties of its previous quantum state. To rebuild the wave function Ψ (up to the precision of an unimportant constant complex factor $e^{i\phi}$), it is necessary to perform *infinite repeated measurements* of the quantum system under the *same initial conditions*. Abstractly, this procedure is equivalent to consider simultaneous measurements over a *quantum statistical ensemble*: such as an infinite set of identical copies of the quantum system, which have been previously prepared under the same experimental procedure². Due to the important role of measurements in the knowledge state of quantum systems, *quantum mechanics is a physical theory that allows us to predict the results of certain experimental measurements taken over a quantum statistical ensemble that it has been previously prepared under certain experimental criteria* (12).

2.2.2 The superposition principle

To explain interference phenomena observed in the double-slit experiments, the wave function $\Psi(\mathbf{q}, t)$ of a quantum system should satisfy the *superposition principle* (12):

$$\Psi(\mathbf{q}, t) = \sum_{\alpha} a_{\alpha} \Psi_{\alpha}(\mathbf{q}, t). \quad (5)$$

Here, $\Psi_{\alpha}(\mathbf{q}, t)$ represents the normalized wave function associated with the α -th independent state. As example, $\Psi_{\alpha}(\mathbf{q}, t)$ could represent the wave function contribution associated with each slit during electron interference experiments; while the modulus $|a_{\alpha}|^2$ of the complex amplitudes a_{α} are proportional to incident beam intensities I_{α} , or equivalently, the probability p_{α} that a given electron crosses through the α -th slit.

² This ensemble definition corresponds to the so-called *pure quantum state*, whose description is performed in terms of the wave function Ψ . A more general extension is the mixed statistical ensemble that corresponds to the so-called *mixed quantum state*, whose description is performed in terms of the *density matrix* $\hat{\rho}$. The consideration of the density matrix is the natural description of quantum statistical mechanics.

Superposition principle is the most important hypothesis with a positive content of quantum theory. In particular, it evidences that dynamical equations of the wave function $\Psi(\mathbf{q}, t)$ should exhibit a *linear character*. By itself, the superposition principle allows to assume linear algebra as the mathematical apparatus of quantum mechanics. Thus, the wave function $\Psi(\mathbf{q}, t)$ can be regarded as a complex vector in a *Hilbert space* \mathcal{H} . Under this interpretation, the superposition formula (5) can be regarded as a decomposition of a vector Ψ in a basis of independent vectors $\{\Psi_\alpha\}$. The normalization of the wave function Ψ can be interpreted as the *vectorial norm*:

$$\|\Psi\|^2 = \int \Psi^*(\mathbf{q}, t)\Psi(\mathbf{q}, t)d\mathbf{q} = \sum_{\alpha\beta} g_{\alpha\beta} a_\alpha^* a_\beta = 1. \quad (6)$$

Here, the matrix elements $g_{\alpha\beta}$ denote the *scalar product* (complex) between different basis elements:

$$g_{\alpha\beta} = \int \Psi_\alpha^*(\mathbf{q}, t)\Psi_\beta(\mathbf{q}, t)d\mathbf{q}, \quad (7)$$

which accounts for the existence of interference effects during the experimental measurements. As expected, the interference matrix, $g_{\alpha\beta}$, is a hermitian matrix, $g_{\alpha\beta} = g_{\beta\alpha}^*$. The basis $\{\Psi_\alpha(\mathbf{q}, t)\}$ is said to be *orthonormal* if their elements satisfy *orthogonality condition*:

$$\int \Psi_\alpha^*(\mathbf{q}, t)\Psi_\beta(\mathbf{q}, t)d\mathbf{q} = \delta_{\alpha\beta}, \quad (8)$$

where $\delta_{\alpha\beta}$ represents Kroneker delta (for a basis with discrete elements) or a Dirac delta functions (for the basis with continuous elements). The basis of independent states is *complete* if any admissible state $\Psi \in \mathcal{H}$ can be represented with this basis. In particular, a basis with independent orthogonal elements is complete if it satisfies the *completeness condition*:

$$\sum_{\alpha} \Psi_\alpha^*(\tilde{\mathbf{q}}, t)\Psi_\alpha(\mathbf{q}, t) = \delta(\tilde{\mathbf{q}} - \mathbf{q}). \quad (9)$$

2.2.3 The correspondence principle

Other important hypothesis of quantum mechanics is the *correspondence principle*. We assume the following suitable statement: the wave-function $\Psi(\mathbf{q}, t)$ can be approximated in the *quasi-classic limit* $\hbar \rightarrow 0$ as follows (12):

$$\Psi(\mathbf{q}, t) \sim \exp[iS(\mathbf{q}, t)/\hbar], \quad (10)$$

where $S(\mathbf{q}, t)$ is the classical action of the system associated with the known Hamilton-Jacobi theory of classical mechanics. Physically, this principle expresses that quantum mechanics contains classical mechanics as an asymptotic theory. At the same time, it states that quantum mechanics should be formulated under the correspondence with classical mechanics. Physically speaking, it is impossible to introduce a consistent quantum mechanics formulation without the consideration of classical notions. Precisely, this is a very consequence of the complementarity between the dynamical description performed in terms of the wave function Ψ and the *space-time classical description* associated with the results of experimental measurements. The completeness of quantum description performed in terms of the wave function Ψ demands both the presence of quantum statistical ensemble and classical objects that play the role of measuring instruments.

Historically, correspondence principle was formally introduced by Bohr in 1920 (16), although he previously made use of it as early as 1913 in developing his model of the atom

(17). According to this principle, quantum description should be consistent with classical description in the limit of large quantum numbers. In the framework of Schrödinger's wave mechanics, this principle appears as a suitable generalization of the so-called *optics-mechanical analogy* (18). In geometric optics, the light propagation is described in the so-called rays approximation. According to the *Fermat's principle*, the ray trajectories extremize the optical length $\ell[\mathbf{q}(s)]$:

$$\ell[\mathbf{q}(s)] = \int_{s_1}^{s_2} n[\mathbf{q}(s)] ds \rightarrow \delta\ell[\mathbf{q}(s)] = 0, \quad (11)$$

which is calculated along the curve $\mathbf{q}(s)$ with fixed extreme points $\mathbf{q}(s_1) = P$ and $\mathbf{q}(s_2) = Q$. Here, $n(\mathbf{q})$ is the refraction index of the optical medium and $ds = |d\mathbf{q}|$. Equivalently, the rays propagation can be described by *Eikonal equation*:

$$|\nabla\varphi(\mathbf{q})|^2 = k_0^2 n^2(\mathbf{q}), \quad (12)$$

where $\varphi(\mathbf{q})$ is the phase of the undulatory function $u(\mathbf{q}, t) = a(\mathbf{q}, t) \exp[-i\omega t + i\varphi(\mathbf{q})]$ in the wave optics, $k_0 = \omega/c$ and c are the modulus of the wave vector and the speed of light in vacuum, respectively. The phase $\varphi(\mathbf{q})$ allows to obtain the wave vector $\mathbf{k}(\mathbf{q})$ within the optical medium:

$$\mathbf{k}(\mathbf{q}) = \nabla\varphi(\mathbf{q}) \rightarrow k(\mathbf{q}) = |\mathbf{k}(\mathbf{q})| = k_0 n(\mathbf{q}), \quad (13)$$

which provides the orientation of the ray propagation:

$$\frac{d\mathbf{q}(s)}{ds} = \frac{\mathbf{k}(\mathbf{q})}{|\mathbf{k}(\mathbf{q})|}. \quad (14)$$

Equation (12) can be derived from the wave equation:

$$n^2(\mathbf{q}) \frac{\partial^2}{c^2 \partial t^2} u(\mathbf{q}, t) = \nabla^2 u(\mathbf{q}, t) \quad (15)$$

considering the approximations $|\partial^2 a(\mathbf{q}, t)/\partial t^2| \ll \omega^2 |a(\mathbf{q}, t)|$ and $|\nabla^2 a(\mathbf{q}, t)| \ll k^2(\mathbf{q}) |a(\mathbf{q}, t)|$. Remarkably, Eikonal equation (12) is equivalent in the mathematical sense to the Hamilton-Jacobi equation for a conservative mechanical system:

$$\frac{1}{2m} |\nabla W(\mathbf{q})|^2 = E - V(\mathbf{q}), \quad (16)$$

where $W(\mathbf{q})$ is the reduced action that appears in the classical action $S(\mathbf{q}, t) = W(\mathbf{q}) - Et$. Analogously, Fresnel's principle is a counterpart of *Maupertuis' principle*:

$$\delta \int \sqrt{2m[E - V(\mathbf{q})]} ds = 0. \quad (17)$$

In quantum mechanics, the optics-mechanics analogy suggests the way that quantum theory asymptotically drops to classical mechanics in the limit $\hbar \rightarrow 0$. Specifically, the total phase $\varphi(\mathbf{q}, t) = \varphi(\mathbf{q}) - \omega t$ of the wave function $\Psi(\mathbf{q}, t) \sim \exp[i\varphi(\mathbf{q}, t)]$ should be proportional to the classical action of Hamilton-Jacobi theory, $\varphi(\mathbf{q}, t) \sim S(\mathbf{q}, t)/\hbar$, consideration that leads to expression (10).

2.2.4 Operators of physical observables and Schrödinger equation

Physical interpretation of the wave function $\Psi(\mathbf{q}, t)$ implies that the expectation value of any arbitrary function $A(\mathbf{q})$ that is defined on the space coordinates \mathbf{q} is expressed as follows:

$$\langle A \rangle = \int |\Psi(\mathbf{q}, t)|^2 A(\mathbf{q}) d\mathbf{q}. \quad (18)$$

For calculating the expectation value of an arbitrary physical observable O , the previous expression should be extended to a *bilinear form* in term of the wave function $\Psi(\mathbf{q}, t)$ (19):

$$\langle O \rangle = \int \Psi^*(\mathbf{q}, t) O(\mathbf{q}, \tilde{\mathbf{q}}, t) \Psi(\tilde{\mathbf{q}}, t) d\mathbf{q} d\tilde{\mathbf{q}}, \quad (19)$$

where $O(\mathbf{q}, \tilde{\mathbf{q}}, t)$ is the kernel of the physical observable O . As already commented, there exist some physical observables, e.g.: the momentum \mathbf{p} , whose determination demands repetitions of measurements in a finite region of the space sufficient for the manifestation of wave properties of the function $\Psi(\mathbf{q}, t)$. Precisely, this type of procedure involves a comparison or correlation between different points of the space $(\mathbf{q}, \tilde{\mathbf{q}})$, which is accounted for by the kernel $O(\mathbf{q}, \tilde{\mathbf{q}}, t)$. Due to the expectation value of any physical observable O is a real number, the kernel $O(\mathbf{q}, \tilde{\mathbf{q}}, t)$ should obey the *hermitian condition*:

$$O^*(\tilde{\mathbf{q}}, \mathbf{q}, t) = O(\mathbf{q}, \tilde{\mathbf{q}}, t). \quad (20)$$

As commented before, superposition principle (5) has naturally introduced the linear algebra on a Hilbert space \mathcal{H} as the mathematical apparatus of quantum mechanics. Using the decomposition of the wave function Ψ into a certain basis $\{\Psi_\alpha\}$, it is possible to obtain the following expressions:

$$\langle O \rangle = \sum_{\alpha\beta} a_\alpha^* O_{\alpha\beta} a_\beta, \quad (21)$$

where:

$$O_{\alpha\beta} = \int \Psi_\alpha^*(\mathbf{q}, t) O(\mathbf{q}, \tilde{\mathbf{q}}, t) \Psi_\beta(\tilde{\mathbf{q}}, t) d\tilde{\mathbf{q}} d\mathbf{q}. \quad (22)$$

Notice that hermitian condition (20) implies the hermitian character of operator matrix elements, $O_{\beta\alpha}^* = O_{\alpha\beta}$. The application of the kernel $O(\mathbf{q}, \tilde{\mathbf{q}}, t)$ over a wave function $\Psi(\mathbf{q}, t)$:

$$\Phi(\mathbf{q}, t) = \int O(\mathbf{q}, \tilde{\mathbf{q}}, t) \Psi(\tilde{\mathbf{q}}, t) d\tilde{\mathbf{q}} \quad (23)$$

yields a new vector $\Phi(\mathbf{q}, t)$ of the Hilbert space, $\Phi(\mathbf{q}, t) \in \mathcal{H}$. Formally, this operation is equivalent to associate each physical observable O with a *linear operator* \hat{O} :

$$\hat{O} \left(\sum_\alpha a_\alpha \Psi_\alpha \right) = \sum_\alpha a_\alpha \hat{O} \Psi_\alpha, \quad (24)$$

where:

$$\hat{O} \Psi(\mathbf{q}, t) \equiv \int O(\mathbf{q}, \tilde{\mathbf{q}}, t) \Psi(\tilde{\mathbf{q}}, t) d\tilde{\mathbf{q}}. \quad (25)$$

This last notation convention allows to rephrase expression (19) for calculating the physical expectation values into the following familiar form:

$$\langle O \rangle = \int \Psi^*(\mathbf{q}, t) \hat{O} \Psi(\mathbf{q}, t) d\mathbf{q}. \quad (26)$$

The application of the physical operator \hat{O} on any element Ψ_β of the orthonormal basis, $\{\Psi_\alpha\}$, can be decomposed into the same basis:

$$\hat{O}\Psi_\beta = \sum_\alpha O_{\alpha\beta}\Psi_\alpha. \quad (27)$$

Moreover, the kernel $O(\tilde{\mathbf{q}}, \mathbf{q}, t)$ can be expressed in this orthonormal basis as follows:

$$O(\tilde{\mathbf{q}}, \mathbf{q}, t) = \sum_{\alpha\beta} \Psi_\alpha(\tilde{\mathbf{q}}, t) O_{\alpha\beta} \Psi_\beta^*(\mathbf{q}, t). \quad (28)$$

Denoting by $T_{m\alpha}$ the transformation matrix elements from the basis $\{\Psi_\alpha\}$ to a new basis $\{\Psi_m\}$:

$$\Psi_\alpha = \sum_m T_{m\alpha} \Psi_m, \quad (29)$$

the operator matrix elements O_{mn} in this new basis can be expressed as follows:

$$O_{mn} = \sum_{\alpha\beta} T_{m\alpha} O_{\alpha\beta} T_{\beta n}^{-1}. \quad (30)$$

Using an appropriate transformation, the operator matrix elements can be expressed into a diagonal form: $O_{mn} = O_m \delta_{mn}$. Such a basis can be regarded as the *proper representation* of the physical operator \hat{O} , which corresponds to the eigenvalues problem:

$$\hat{O}\Psi_m(\mathbf{q}, t) = O_m \Psi_m(\mathbf{q}, t). \quad (31)$$

The eigenvalues O_m conform the *spectrum* of the physical operator \hat{O} , that is, its admissible values observed in the experiment. On the other hand, the set of eigenfunctions $\{\Psi_m\}$ can be used to introduce a basis in the Hilbert space \mathcal{H} , whenever it represents a complete set of functions. Using this basis of eigenfunctions, it is possible to obtain some remarkable results. For example, the expectation value of physical observable O can be expressed into the ordinary expression:

$$\langle O \rangle = \sum_m O_m p_m, \quad (32)$$

where $p_m = |a_m|^2$ is the probability of the m -th eigenstate. Using the hermitian character of any physical operator $\hat{O}^+ = \hat{O}$, it is possible to obtain the following result:

$$(O_m - O_n) \int \Psi_m^*(\mathbf{q}, t) \Psi_n(\mathbf{q}, t) d\mathbf{q} = 0. \quad (33)$$

If $O_m \neq O_n$, the corresponding eigenfunctions $\Psi_m(\mathbf{q}, t)$ and $\Psi_n(\mathbf{q}, t)$ are *orthogonal*. Additionally, if two physical operators \hat{A} and \hat{B} possesses the same spectrum of eigenfunctions, the commutator of these operators:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad (34)$$

identically vanishes:

$$[\hat{A}, \hat{B}] = 0. \quad (35)$$

Such an operational identity is shown as follows. Considering a general function $\Psi \in \mathcal{H}$ and its representation using the complete orthonormal basis $\{\Psi_m\}$:

$$\Psi = \sum_m a_m \Psi_m, \quad (36)$$

one obtains the following relation:

$$[\hat{A}, \hat{B}]\Psi = \sum_m a_m (\hat{A}\hat{B} - \hat{B}\hat{A})\Psi_m = \sum_m a_m (A_m B_m - B_m A_m)\Psi_m = 0. \quad (37)$$

Clearly, a complete orthonormal basis $\{\Psi_m\}$ in the Hilbert space \mathcal{H} is conformed by the eigenfunctions of all admissible and independent physical operators that commute among them.

According to expression (18), the operators of spatial coordinates \mathbf{q} and their functions $A(\mathbf{q})$ are simply given by these coordinates, $\hat{\mathbf{q}} = \mathbf{q}$ and $\hat{A}(\mathbf{q}) = A(\mathbf{q})$. The introduction of physical operators in quantum mechanics is precisely based on the correspondence with classical mechanics. Relevant examples are the physical operators of energy and momentum (19):

$$\hat{E} = i\hbar \frac{\partial}{\partial t} \text{ and } \hat{\mathbf{p}} = -i\hbar \nabla. \quad (38)$$

Clearly, the wave function of the free microparticle (4) is just the eigenfunction of these operators. Using the quasi-classical expression of the wave function (10), these operators drop to their classical definitions in the Hamilton-Jacobi theory (18):

$$\hat{\mathbf{p}}\Psi(\mathbf{q}, t) \sim \hat{\mathbf{p}} \exp[iS(\mathbf{q}, t)/\hbar] \Rightarrow \mathbf{p} = \nabla S(\mathbf{q}, t), \quad (39)$$

$$\hat{E}\Psi(\mathbf{q}, t) \sim \hat{E} \exp[iS(\mathbf{q}, t)/\hbar] \Rightarrow -\frac{\partial}{\partial t} S(\mathbf{q}, t) = H(\mathbf{q}, \mathbf{p}, t), \quad (40)$$

where $H(\mathbf{q}, \mathbf{p}, t)$ is the Hamiltonian, which represents the energy E in the case of a conservative mechanical system $H(\mathbf{q}, \mathbf{p}, t) = H(\mathbf{q}, \mathbf{p}) = E$. In the framework of Hamilton-Jacobi theory, the system dynamics is described by the following equation:

$$\frac{\partial}{\partial t} S(\mathbf{q}, t) + H(\mathbf{q}, \nabla S(\mathbf{q}, t), t). \quad (41)$$

Its quantum mechanics counterpart is the well-known *Schrödinger equation* (19):

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{q}, t) = \hat{H}\Psi(\mathbf{q}, t) \quad (42)$$

where $\hat{H} = H(\mathbf{q}, \hat{\mathbf{p}}, t)$ is the corresponding operator of the system Hamiltonian.

2.3 Derivation of complementary relations

Let us introduce the scalar z -product between two arbitrary vectors Ψ_1 and Ψ_2 of the Hilbert space \mathcal{H} :

$$\Psi_1 \otimes_z \Psi_2 = \frac{1}{2} z \langle \Psi_1 | \Psi_2 \rangle + \frac{1}{2} z^* \langle \Psi_2 | \Psi_1 \rangle, \quad (43)$$

where $\langle \Psi_1 | \Psi_2 \rangle$ denotes:

$$\langle \Psi_1 | \Psi_2 \rangle \equiv \int \Psi_1^*(\mathbf{q}, t) \Psi_2(\mathbf{q}, t) d\mathbf{q}. \quad (44)$$

The scalar z -product is always real for any Ψ_1 and $\Psi_2 \in \mathcal{H}$ and obeys the following properties:

1. *Linearity*:

$$\Psi \otimes_z (\Psi_1 + \Psi_2) = \Psi \otimes_z \Psi_1 + \Psi \otimes_z \Psi_2, \quad (45)$$

2. *Homogeneity:*

$$\Psi_1 \otimes_z (w\Psi_2) = \Psi_1 \otimes_{zw} \Psi_2, \quad (46)$$

3. *z-Symmetry:*

$$\Psi_1 \otimes_z \Psi_2 = \Psi_2 \otimes_{z^*} \Psi_1 \quad (47)$$

4. *Nonnegative definition:* if $\Re(z) > 0$ then:

$$\Psi \otimes_z \Psi \geq 0 \text{ and } \Psi \otimes_z \Psi = 0 \Rightarrow \Psi = 0. \quad (48)$$

Denoting as $\Psi_1 \otimes \Psi_2$ the case $z = 1$, it is easy to obtain the following relation:

$$\Psi \otimes_z \Psi = \Re(z)\Psi \otimes \Psi = \Re(z) \|\Psi\|^2, \quad (49)$$

where $\|\Psi\|^2 = \langle \Psi | \Psi \rangle$ denotes the *norm of the vector* $\Psi \in \mathcal{H}$. Considering $w = |w|e^{i\phi}$, the inequality

$$(\Psi_1 + w\Psi_2) \otimes (\Psi_1 + w\Psi_2) \geq 0 \quad (50)$$

can be rewritten as follows:

$$\Psi_1 \otimes \Psi_1 + |w|^2 \Psi_2 \otimes \Psi_2 + 2|w| \Psi_1 \otimes_{e^{i\phi}} \Psi_2 \geq 0. \quad (51)$$

The nonnegative definition of the previous expression demands the applicability of the following inequality:

$$\|\Psi_1\|^2 \|\Psi_2\|^2 \geq \left(\Psi_1 \otimes_{e^{i\phi}} \Psi_2 \right)^2, \quad (52)$$

which represents a special form of the Cauchy-Schwartz inequality. Considering two physical operators \hat{A} and \hat{B} with vanishing expectation values $\langle A \rangle = \langle B \rangle = 0$, and considering $\Psi_1 = \hat{A}\Psi$ and $\Psi_2 = \hat{B}\Psi$, it is possible to obtain the following expression:

$$\Psi_1 \otimes_{e^{i\phi}} \Psi_2 = \frac{1}{2} \cos \phi \langle C_A \rangle - \frac{1}{2} \sin \phi \langle C \rangle, \quad (53)$$

where $\langle C_A \rangle$ and $\langle C \rangle$ are the expectation values of physical operators \hat{C}_A and \hat{C} :

$$\hat{C}_A = \{ \hat{A}, \hat{B} \} = \hat{A}\hat{B} + \hat{B}\hat{A} \text{ and } i\hat{C} = [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}. \quad (54)$$

Introducing the *statistical uncertainty* $\Delta O = \sqrt{\langle (O - \langle O \rangle)^2 \rangle}$ of the physical observable O , inequality (52) can be rewritten as follows:

$$\Delta A \Delta B \geq \frac{1}{2} |\cos \phi \langle C_A \rangle - \sin \phi \langle C \rangle|. \quad (55)$$

Relevant particular cases of the previous result are the following inequalities:

$$\Delta A \Delta B \geq \frac{1}{2} |\langle C_A \rangle|, \quad \Delta A \Delta B \geq \frac{1}{2} |\langle C \rangle|, \quad (56)$$

$$\Delta A \Delta B \geq \frac{1}{2} \sqrt{\langle C_A \rangle^2 + \langle C \rangle^2}. \quad (57)$$

Accordingly, the product of statistical uncertainties of two physical observables A and B are inferior bounded by the commutator \hat{C} , or the anti-commutator \hat{C}_A of their respective operators. The commutator form of Eq.(56) was firstly obtained by Robertson in 1929 (20), who generalizes a particular result derived by Kennard (21):

$$\Delta q^i \Delta p_i \geq \frac{1}{2} \hbar, \quad (58)$$

using the commutator relations:

$$[\hat{q}^i, \hat{p}_j] = i\delta_j^i \hbar. \quad (59)$$

The inequality of Eq.(57) was finally obtained by Schrödinger (22) and it is now referred to as *Robertson-Schrodinger inequality*. Historically, Kennard's result in (58) was the first rigorous mathematical demonstration about the uncertainty relation between coordinates and momentum, which provided evidences that *Heisenberg's uncertainty relations* can be obtained as direct consequences of statistical character of the algebraic apparatus of quantum mechanics.

3. Relevant inequalities in classical probability theory

Hereafter, let us consider a generic classical distribution function:

$$dp(I|\theta) = \rho(I|\theta)dI \quad (60)$$

where $I = (I^1, I^2, \dots, I^m)$ denotes a set of continuous stochastic variables driven by a set $\theta = (\theta^1, \theta^2, \dots, \theta^m)$ of the control parameters. Let us denote by \mathcal{M}_θ the compact manifold constituted by all admissible values of the variables I that are accessible for a fixed $\theta \in \mathcal{P}$, where \mathcal{P} is the compact manifold of all admissible values of control parameters θ . Moreover, let us admit that the probability density $\rho(I|\theta)$ obeys some general mathematical conditions as normalization, differentiability, as well as regular boundary conditions as:

$$\lim_{I \rightarrow I_b} \rho(I|\theta) = \lim_{I \rightarrow I_b} \frac{\partial}{\partial I^i} \rho(I|\theta) = 0, \quad (61)$$

where I_b is any point located at the boundary $\partial\mathcal{M}_\theta$ of the manifold \mathcal{M}_θ . The parametric family of distribution functions of Eq.(60) can be analyzed by two different perspectives:

- The study of fluctuating behavior of stochastic variables $I \in \mathcal{M}_\theta$, which is the main interest of *fluctuation theory*;
- The analysis of the relationship between this fluctuating behavior and the external influence described in terms of parameters $\theta \in \mathcal{P}$, which is the interest of *inference theory*.

3.1 Fluctuation theory

The probability density $\rho(I|\theta)$ can be employed to introduce the *generalized differential forces* $\eta_i(I|\theta)$ as follows (8; 9):

$$\eta_i(I|\theta) = -\frac{\partial}{\partial I^i} \log \rho(I|\theta). \quad (62)$$

By definition, the quantities $\eta_i(I|\theta)$ vanish in those stationary points \bar{I} where the probability density $\rho(I|\theta)$ exhibits its local maxima or its local minima. In statistical mechanics, the global (local) maximum of the probability density is commonly regarded as a stable (metastable)

equilibrium configuration. These notable points can be obtained from the maximization of the logarithm of the probability density $\rho(I|\theta)$, which leads to the following *stationary and stability equilibrium conditions*:

$$\eta_i(\bar{I}|\theta) = 0, \text{ and } \frac{\partial}{\partial I^i} \eta_j(\bar{I}|\theta) \succ 0, \quad (63)$$

where the notation $A_{ij} \succ 0$ indicates the positive definition of the matrix A_{ij} . In general, the differential generalized forces $\eta_i(I|\theta)$ characterize the deviation of a given point $I \in \mathcal{M}_\theta$ from these local equilibrium configurations. As stochastic variables, the differential generalized forces $\eta_i(I|\theta)$ obey the following fluctuation theorems (8; 9):

$$\langle \eta_i(I|\theta) \rangle = 0, \left\langle \frac{\partial}{\partial I^i} \eta_j(I|\theta) \right\rangle = \langle \eta_i(I|\theta) \eta_j(I|\theta) \rangle, \langle \eta_i(I|\theta) \delta I^j \rangle = \delta_i^j, \quad (64)$$

where δ_i^j is the Kronecker delta. These fluctuation theorems are directly derived from the following identity:

$$\left\langle \frac{\partial}{\partial I^i} A(I|\theta) \right\rangle = \langle \eta_i(I|\theta) A(I|\theta) \rangle \quad (65)$$

substituting the cases $A(I|\theta) = 1, I^i$ and η_i , respectively. Here, $A(I)$ is a differentiable function defined on the continuous variables I with definite expectation values $\langle \partial A(I|\theta) / \partial I^i \rangle$ that obeys the following boundary condition:

$$\lim_{I \rightarrow I_\theta} A(I) \rho(I|\theta) = 0. \quad (66)$$

Moreover, equation (65) follows from the integral expression:

$$\int_{\mathcal{M}_\theta} \frac{\partial v^j(I|\theta)}{\partial I^i} \rho(I|\theta) dI = - \int_{\mathcal{M}_\theta} v^j(I|\theta) \frac{\partial \rho(I|\theta)}{\partial I^i} dI + \oint_{\partial \mathcal{M}_\theta} \rho(I|\theta) v^j(I|\theta) \cdot d\Sigma_j,$$

that is derived from the *intrinsic exterior calculus* of the manifold \mathcal{M}_θ and the imposition of the constraint $v^j(I|\theta) \equiv \delta_i^j A(I|\theta)$. Since the self-correlation matrix $M_{ij}(\theta) = \langle \eta_i(I|\theta) \eta_j(I|\theta) \rangle$ is always a positive definite matrix, the first and second identities are counterpart expressions of the stationary and stability equilibrium conditions of Eq.(63) in the form of statistical expectation values. The third identity shows the statistical independence among the variable I^i and a generalized differential force component $\eta_j(I|\theta)$ with $j \neq i$, as well as the existence of a certain *statistical complementarity* between I^i and its conjugated generalized differential force $\eta_i(I|\theta)$. Using the Cauchy-Schwartz inequality $\langle \delta x \delta y \rangle^2 \leq \langle \delta x^2 \rangle \langle \delta y^2 \rangle$, one obtains the following *uncertainty-like relation* (8; 9):

$$\Delta I^i \Delta \eta_i \geq 1, \quad (67)$$

where $\Delta x = \sqrt{\langle \delta x^2 \rangle}$ denotes the standard deviation of the quantity x . The previous result is improved by the following inequality:

$$\langle \delta I^i \delta I^j \rangle - M^{ij}(\theta) \succ 0, \quad (68)$$

which puts a lower bound to the self-correlation matrix $\tilde{C}^{ij} = \langle \delta I^i \delta I^j \rangle$ of the stochastic variables I . This result can be directly obtained from the positive definition of the self-correlation matrix $Q^{ij}(\theta) = \langle \delta q^i \delta q^j \rangle$, where $\delta q^i = \delta I^i - M^{ij}(\theta)\eta_j(I|\theta)$, with $M^{ij}(\theta)$ being the inverse of the self-correlation matrix $M_{ij}(\theta) = \langle \eta_i(I|\theta)\eta_j(I|\theta) \rangle$.

3.2 Inference theory

Inference theory addresses the problem of deciding how well a set of outcomes $\mathcal{I} = (I_1, I_2, \dots, I_s)$, which is obtained from s independent measurements, fits to a proposed probability distribution $dp(I|\theta) = \rho(I|\theta)dI$. If the probability distribution is characterized by one or more parameters $\theta = (\theta^1, \theta^2, \dots, \theta^m)$, this problem is equivalent to infer their values from the observed outcomes I . To make inferences about the parameters θ , one constructs estimators, i.e., functions $\hat{\theta}^\alpha(\mathcal{I}) = \hat{\theta}^\alpha(I_1, I_2, \dots, I_s)$ of the outcomes of m independent repeated measurements (10; 11). The values of these functions represent the best guess for θ . Commonly, there exist several criteria imposed on estimators to ensure that their values constitute good estimates for θ , such as unbiasedness, $\langle \hat{\theta}^\alpha \rangle = \theta^\alpha$, efficiency, $\langle (\hat{\theta}^\alpha - \theta^\alpha)^2 \rangle \rightarrow \text{minimum}$, etc. One of the most popular estimators employed in practical applications are the maximal likelihood estimators $\hat{\theta}_{ml}$ (10), which are obtained introducing the likelihood function:

$$\varrho(\mathcal{I}|\theta) = \rho(I_1|\theta)\rho(I_2|\theta) \dots \rho(I_m|\theta) \quad (69)$$

and demanding the condition $\varrho(\mathcal{I}|\hat{\theta}_{ml}) \rightarrow \text{maximum}$. This procedure leads to the following stationary and stability conditions:

$$v_\alpha(\mathcal{I}|\hat{\theta}_{ml}) = 0, \quad \frac{\partial}{\partial \theta^\alpha} v_\beta(\mathcal{I}|\hat{\theta}_{ml}) \succ 0. \quad (70)$$

where the quantities $v_\alpha(\mathcal{I}|\theta)$ are referred to in the literature as the score vector components:

$$v_\alpha(\mathcal{I}|\theta) = -\frac{\partial}{\partial \theta^\alpha} \log \varrho(\mathcal{I}|\theta). \quad (71)$$

As stochastic quantities, the score vector components $v_\alpha(\mathcal{I}|\theta)$ obey the following identities:

$$\langle v_\alpha(\mathcal{I}|\theta) \rangle = 0, \quad \left\langle \frac{\partial}{\partial \theta^\alpha} v_\beta(\mathcal{I}|\theta) \right\rangle = \langle v_\alpha(\mathcal{I}|\theta)v_\beta(\mathcal{I}|\theta) \rangle, \quad \langle \hat{\theta}^\alpha(\mathcal{I})v_\beta(\mathcal{I}|\theta) \rangle = -\delta_{\beta}^\alpha, \quad (72)$$

where $\hat{\theta}^\alpha(\mathcal{I})$ represents an unbiased estimator for the α -th parameter θ^α . Moreover, expectation values $\langle A(\mathcal{I}) \rangle$ are defined as follows:

$$\langle A(\mathcal{I}) \rangle = \int_{\mathcal{M}_\theta^s} A(\mathcal{I})\varrho(\mathcal{I}|\theta)d\mathcal{I}, \quad (73)$$

where $d\mathcal{I} = \prod_i dI_i$ and $\mathcal{M}_\theta^s = \mathcal{M}_\theta \otimes \mathcal{M}_\theta \dots \mathcal{M}_\theta$ (s times the external product of the manifold \mathcal{M}_θ). The fluctuation expressions (72) are derived from the mathematical identity:

$$\langle \partial_\alpha A(\mathcal{I}|\theta) \rangle - \partial_\alpha \langle A(\mathcal{I}|\theta) \rangle = \langle A(\mathcal{I}|\theta)v_\alpha(\mathcal{I}|\theta) \rangle, \quad (74)$$

which is obtained from Eq.(73) taking the partial derivative $\partial_\alpha = \partial/\partial\theta^\alpha$. The first two identities can be regarded as the stationary and stability conditions of maximal likelihood estimators of Eq.(70) written in term of statistical expectation values. Using the

Inference theory	Fluctuation theory
score vector components: $v_\alpha(\mathcal{I} \theta) = -\frac{\partial}{\partial \theta^\alpha} \log \varrho(\mathcal{I} \theta)$	generalized differential forces: $\eta_i(I \theta) = -\frac{\partial}{\partial I^i} \log \rho(I \theta)$
conditions for likelihood estimators: $v_\alpha(\mathcal{I} \hat{\theta}_{ml}) = 0, \frac{\partial}{\partial \theta^\alpha} v_\beta(\mathcal{I} \hat{\theta}_{ml}) \succ 0$	thermodynamic equilibrium conditions: $\eta_i(\bar{I} \theta) = 0, \frac{\partial}{\partial I^i} \eta_j(\bar{I} \theta) \succ 0$
inference fluctuation theorems: $\langle v_\alpha(\mathcal{I} \theta) \rangle = 0$ $\left\langle \frac{\partial}{\partial \theta^\alpha} v_\beta(\mathcal{I} \theta) \right\rangle = \left\langle v_\alpha(\mathcal{I} \theta) v_\beta(\mathcal{I} \theta) \right\rangle$ $\left\langle v_\alpha(\mathcal{I} \theta) \delta \hat{\theta}^\beta \right\rangle = -\delta_\alpha^\beta$	equilibrium fluctuation theorems: $\langle \eta_i(I \theta) \rangle = 0$ $\left\langle \frac{\partial}{\partial I^i} \eta_j(I \theta) \right\rangle = \left\langle \eta_i(I \theta) \eta_j(I \theta) \right\rangle$ $\left\langle \eta_i(I \theta) \delta I^j(I \theta) \right\rangle = \delta_i^j$

Table 1. Fluctuation theory and inference theory can be regarded as dual counterpart statistical approaches.

Cauchy-Schwartz inequality, the third relation states a strong fluctuation relation between unbiased estimators and the score vector components:

$$\Delta v_\alpha \Delta \hat{\theta}^\alpha \geq 1, \quad (75)$$

which can be generalized by the following inequality:

$$\left\langle \delta \hat{\theta}^\alpha \delta \hat{\theta}^\beta \right\rangle - g_F^{\alpha\beta}(\theta) \succ 0. \quad (76)$$

Here, $g_F^{\alpha\beta}(\theta)$ denotes the inverse matrix of the Fisher's inference matrix (10):

$$g_{\alpha\beta}^F(\theta) = \left\langle v_\alpha(\mathcal{I}|\theta) v_\beta(\mathcal{I}|\theta) \right\rangle. \quad (77)$$

Eq.(76) is the famous *Cramer-Rao theorem* of inference theory (11), which puts a lower bound to the efficiency of any unbiased estimators $\hat{\theta}^\alpha$.

As clearly shown in Table 1, fluctuation theory and inference theory can be regarded as *dual counterpart statistical approaches* (9). In fact, there exists a direct correspondence among their respective definitions and theorems. As naturally expected, inequalities of Eqs.(67) and (75) could be employed to introduce *uncertainty relations* in a given physical theory with a statistical mathematical apparatus.

4. Complementarity in classical statistical mechanics

Previously, many specialists proposed different attempts to support the existence of an *energy-temperature complementarity* inspired on Bohr's arguments referred to in the introductory section. Relevant examples of these attempts were proposed by Rosenfeld (23), Mandelbrot (24), Gilmore (25), Lindhard (26), Lavenda (27), Schölg (28), among other authors. Remarkably, the versions of this relation which have appeared in the literature give different interpretations of the uncertainty in temperature $\Delta(1/T)$ and often employ widely different theoretical frameworks, ranging from statistical thermodynamics to modern theories of *statistical inference*. Despite of all devoted effort, this work has not led to a consensus in the literature, as clearly discussed in the most recent review by J. Uffink and J. van Lith (6).

An obvious objection is that the mathematical structure of quantum theories is radically different from that of classical physical theories. In fact, classical theories are not developed

using an *operational formulation*. Remarkably, the previous section evidences that any physical theory with a classical statistical apparatus could support the existence of quantities with a complementary character. Let us analyze the consequences of the uncertainty-like inequalities (67) and (75) in the question about the energy-temperature complementarity in the framework of classical statistical mechanics.

4.1 Energy-temperature complementarity in the framework of inference theory

Mandelbrot was the first to propose an inference interpretation of the Bohr's hypotheses about the *energy-temperature complementarity* (29). Starting from the *canonical ensemble* (CE):

$$dp_{CE}(E|\beta) = \exp(-\beta E/k_B) \Omega(E)dE/Z(\beta), \quad (78)$$

where $\beta = 1/T$, and applying the Cramer-Rao theorem (75), this author obtains the following uncertainty-like inequality:

$$\Delta\hat{\beta}\Delta E \geq k_B, \quad (79)$$

where $\Delta\hat{\beta}$ is just the uncertainty of the inverse temperature parameter β associated with its determination via an inferential procedure from a single measurement ($s = 1$), while ΔE is the statistical uncertainty of the energy. This type of inference interpretation of uncertainty relations can be extended in the framework of *Boltzmann-Gibbs distributions* (BG):

$$dp_{BG}(E, X|\beta, \xi) = \exp[-(\beta E + \xi X)/k_B] \Omega(E, X)dE/Z(\beta, \xi), \quad (80)$$

to the other pairs of conjugated thermodynamic variables:

$$\Delta\hat{\xi}\Delta X \geq k_B, \quad (81)$$

where $\xi = \beta Y$. Here, X represents a generalized displacement (volume V , magnetization M , etc.) while Y is its conjugated generalized force (pressure p , magnetic field H , etc.). Nowadays, this type of inference arguments have been also employed in modern interpretations of quantum uncertainty relations (30–32).

There exist many attempts in the literature to support the energy-temperature complementarity starting from conventional statistical ensembles as (78) or (80), which are reviewed by Uffink and van Lith in Ref.(6). As already commented by these authors, the inequality (79) cannot be taken as a proper uncertainty relation. In fact, it is impossible to reduce to zero the energy uncertainty $\Delta E \rightarrow 0$ to observe an indetermination of the inverse temperature $\Delta\hat{\beta} \rightarrow \infty$ because ΔE is *fixed* in the canonical ensemble (78). Consequently, the present inference arguments are useless to support the existence of a complementarity between *thermal contact* and *energetic isolation*, as it was originally suggested by Bohr. In our opinion, all these attempts are condemned to fail due to a common misunderstanding of the *temperature concept*.

4.2 Remarks on the temperature notion

Many investigators, including Bohr (3), Landau (5) and Kittel (33), assumed that a *definite temperature can only be attribute to a system when it is put in thermal contact with a heat bath*. Although this is the temperature notion commonly employed in thermal physics, this viewpoint implies that the temperature of an isolated system is *imperfectly defined*. This opinion is explicitly expressed in the last paragraph of section §112 of the known Landau & Lifshitz treatise (5). By itself, this idea is *counterfactual*, since it could not be possible to attribute a definite temperature for the system acting as a *heat reservoir* when it is put into *energetic*

isolation. Conversely, the temperature notion of an isolated system admits an unambiguous definition in terms of the famous *Boltzmann's interpretation of thermodynamic entropy*:

$$S = k_B \log W \rightarrow \frac{1}{T} = \frac{\partial S}{\partial E}, \quad (82)$$

where W is the number of microstates compatible with a given macroscopic configuration, e.g.: $W = Sp[\delta(E - \mathcal{H})] \epsilon_0$, with ϵ_0 being a small energy constant that makes W a dimensionless quantity. One realizes after revising the Gibbs' derivation of canonical ensemble (78) from the microcanonical basis that the temperature T appearing as a parameter in the canonical distribution (78) is just the *microcanonical temperature* (82) of the heat reservoir when its size N is sent to the thermodynamic limit $N \rightarrow \infty$. Although such a parameter characterizes the internal conditions of the heat reservoir and its thermodynamic influence on the system under consideration, the same one cannot provide a correct definition for the internal temperature of the system. While the difference between the temperature appearing in the canonical ensemble (78) and the one associated with the microcanonical ensemble (82) is irrelevant in most of everyday practical situations involving *extensive systems*, this is not the case of *small systems*. In fact, microcanonical temperature (82) appears as the only way to explain the existence of *negative heat capacities* $C < 0$:

$$\frac{\partial}{\partial E} \left(\frac{1}{T} \right) = -\frac{1}{T^2 C} \Rightarrow C = - \left(\frac{\partial S}{\partial E} \right)^2 / \left(\frac{\partial^2 S}{\partial E^2} \right) \quad (83)$$

through the *convex character* of the entropy (34), $\partial^2 S / \partial E^2 > 0$. Analyzing the microcanonical notion of temperature (82), one can realize that *only a macroscopic system has a definite temperature into conditions of energetic isolation*. According to this second viewpoint, the system energy E and temperature T cannot manifest a complementary relationship. However, a careful analysis reveals that this preliminary conclusion is *false*.

According to definition (82), temperature is a concept with *classical* and *statistical* relevance. Temperature is a classical notion because of the entropy S should be a *continuous function* on the system energy E . In the framework of quantum systems, this requirement demands the validity of the *continuous approximation* for the system density of states $\Omega(E) = Sp[\delta(E - \hat{\mathcal{H}})]$. Those quantum systems unable to satisfy this last requirement cannot support an *intrinsic value of temperature* T . By itself, this is the main reason why the temperature of thermal physics is generally assumed in the framework of quantum theories. On the other hand, temperature manifests a statistical relevance because of its definition demands the notion of *statistical ensemble*: a set of identical copies of the system compatible with the given macroscopic states. Although it is possible to apply definition (82) to predict temperature $T(E)$ as a function on the system energy E , the practical determination of energy-temperature relation is restricted by the statistical relevance of temperature. In the framework of thermodynamics, the determination of temperature T and the energy E , as well as other conjugated thermodynamic quantities, is based on the interaction of this system with a *measuring instruments*, e.g.: a thermometer, a barometer, etc. Such experimental measurements always involve an uncontrollable perturbation of the initial internal state of the system, which means that thermodynamic quantities as energy E and temperature T are only determined in an imperfect way.

4.3 Energy-temperature complementarity in the framework of fluctuation theory

To arrive at a proper uncertainty relation among thermodynamic variables, it is necessary to start from a general equilibrium situation where the external influence acting on the system under analysis can be controlled, *at will*, by the observer. In classical fluctuation theory, as example, the specific form of the distribution function $dp(I|\theta)$ is taken from the Einstein's postulate (5):

$$dp(I|\theta) = A \exp [S(I|\theta)/k_B] dI, \quad (84)$$

which describes the fluctuating behavior of a closed system with total entropy $S(I|\theta)$. Let us admit that the system under analysis and the measuring instrument conform a closed system. The separability of these two systems admits the additivity of the total entropy $S(I|\theta) = S(I) + S^m(I|\theta)$, where $S^m(I|\theta)$ and $S(I)$ are the contributions of the measuring instrument and the system, respectively.

For convenience, it is worth introducing the *generalized differential operators* $\hat{\eta}_i$

$$\hat{\eta}_i = -k_B \frac{\partial}{\partial I^i} \rightarrow \hat{\eta}_i \rho(I|\theta) = \eta_i(I|\theta) \rho(I|\theta), \quad (85)$$

which act over the probability density $\rho(I|\theta)$ associated with the statistical ensemble (84), providing in this way the difference $\eta_i(I|\theta)$ of the generalized forces $\zeta = (\beta, \zeta)$:

$$\eta_i(I|\theta) = \zeta_i^m - \zeta_i \quad (86)$$

between the system and the measuring instrument:

$$\zeta_i = \frac{\partial S(I)}{\partial I^i} \text{ and } \zeta_i^m = -\frac{\partial S^m(I|\theta)}{\partial I^i}. \quad (87)$$

Clearly, the vanishing of the expectation values $\langle \eta_i(I|\theta) \rangle$ drop to the known *thermodynamic equilibrium conditions*:

$$\langle \zeta_i^m \rangle = \langle \zeta_i \rangle, \quad (88)$$

which are written in the form of *statistical expectation values*. In particular, the *condition of thermal equilibrium* is expressed as follows:

$$\left\langle \frac{1}{T} \right\rangle = \left\langle \frac{1}{T^m} \right\rangle, \quad (89)$$

where T and T^m are the temperatures of the system and the measuring instrument (thermometer), respectively. Analogously, the *condition of mechanical equilibrium*:

$$\left\langle \frac{p}{T} \right\rangle = \left\langle \frac{p^m}{T^m} \right\rangle, \quad (90)$$

where p and p^m are the internal pressures of the system and its measuring instrument (barometer). The application of inequality (67) leads to a special interpretation of the notion of *complementarity between conjugated thermodynamic quantities*:

$$\Delta(\zeta_i^m - \zeta_i) \Delta I^i \geq k_B. \quad (91)$$

Particular examples of these inequalities are the *energy-temperature uncertainty relation* (8):

$$\Delta(1/T - 1/T^m) \Delta E \geq k_B, \quad (92)$$

and the *volume-pressure uncertainty relation*:

$$\Delta(p/T - p^m/T^m)\Delta V \geq k_B. \quad (93)$$

These inequalities express *the impossibility to perform an exact experimental determination of conjugated thermodynamic variables* (e.g.: energy E and temperature T or volume V and pressure p , etc.) *using any experimental procedure based on the thermodynamic equilibrium with a measuring instrument*. Conversely to inference uncertainty relations (79) and (81), the system statistical uncertainties ΔE and ΔV can now be modified *at will* changing the experimental setup, that is, modifying the properties of the measuring instrument.

4.4 Analogies between quantum mechanics and classical statistical mechanics

A simple comparison between classical statistical mechanics and quantum mechanics involves several analogies between these statistical theories (see in Table 2). Physical theories as classical mechanics and thermodynamics assume a simultaneous definition of complementary variables like the coordinate and the momentum (\mathbf{q}, \mathbf{p}) or the energy and the inverse temperature $(E, 1/T)$. A different situation is found in those applications where the relevant constants as the quantum of action \hbar or the Boltzmann's constant k_B are not so small. According to uncertainty relations shown in equations (3) and (92), the thermodynamic state $(E, 1/T)$ of a small thermodynamic system is badly defined in an analogous way that a quantum system cannot support the classical notion of particle trajectory $[\mathbf{q}(t), \mathbf{p}(t)]$.

Apparently, uncertainty relations can be associated with the *coexistence of variables with different relevance* in a statistical theory. In one hand, we have the variables parameterizing the *results of experimental measurements*: space-time coordinates (t, \mathbf{q}) or the mechanical macroscopic observables $I = (I^i)$. On the other hand, we have their conjugated variables associated with the *dynamical description*: the energy-momentum (E, \mathbf{p}) or the generalized differential forces $\eta = (\eta_i)$. These variables control the respective deterministic dynamics: while the energy E and the momentum \mathbf{p} constrain the trajectory $\mathbf{q}(t)$ of a classical mechanic system, the inverse temperature differences, $\eta = 1/T^m - 1/T$, drives the dynamics of the system energy $E(t)$ (i.e.: the energy interchange) and its tendency towards the equilibrium. Similarly, the experimental determination of these dynamical variables demands the consideration of many repeated measurements due to their explicit statistical significance in the framework of their respective statistical theories.

According to the comparison presented in Table 2, the classical action $S(\mathbf{q}, t)$ and the thermodynamic entropy $S(I|\theta)$ can be regarded as two counterpart statistical functions. Interestingly, while the expression (10) describing the relation between the wave function $\Psi(\mathbf{q}, t)$ and the classical action $S(\mathbf{q}, t)$ is simply an asymptotic expression applicable in the quasi-classic limit where $S(\mathbf{q}, t) \gg \hbar$, Einstein's postulate (84) is conventionally assumed as an *exact expression* in classical fluctuation theory. The underlying analogy suggests that Einstein's postulate (84) should be interpreted as an asymptotic expression obtained in the limit $S(I|\theta) \gg k_B$ of a *more general statistical mechanics theory*. This requirement is always satisfied in conventional applications of classical fluctuation theory, which deal with the small fluctuating behavior of large thermodynamic systems. Accordingly, this important hypothesis of classical fluctuation theory should lost its applicability in the case of small thermodynamic systems. In the framework of such a general statistical theory, Planck's constant k_B could be regarded as the *quantum of entropy*.

Classical mechanics provides a precise description for the systems with large quantum numbers, or equivalently, in the limit $\hbar \rightarrow 0$. Similarly, thermodynamics appears as a suitable

Comparison criterium	Quantum mechanics	Classical statistical mechanics
parametrization	space-time coordinates (t, \mathbf{q})	mechanical macroscopic observables $I = (I^i)$
probabilistic description	wave function $\psi(\mathbf{q}, t)$	distribution function $dp(I \theta) = \rho(I \theta) dI$
relevant physical hypothesis	<i>Correspondence principle:</i> $\psi(\mathbf{q}, t) \sim \exp[iS(\mathbf{q}, t)/\hbar]$, where $S(\mathbf{q}, t)$ is the action	Einstein's postulate: $\rho(I \theta) \sim \exp[S(I \theta)/k_B]$, where $S(I \theta)$ is the entropy
evolution	dynamical conservation laws	tendency towards thermodynamic equilibrium
conjugated variables	energy $E = \partial S(\mathbf{q}, t) / \partial t$ momenta $\mathbf{p} = \partial S(\mathbf{q}, t) / \partial \mathbf{q}$	differential forces $\eta_i = \partial S(I \theta) / \partial I^i$
complementary quantities	(\mathbf{q}, t) versus (\mathbf{p}, E)	I^i versus η_i
operator representation	$\hat{q}^i = q^i$ and $\hat{p}_i = -i\hbar \frac{\partial}{\partial q^i}$	$\hat{I}^i = I^i$ and $\hat{\eta}_i = -k_B \frac{\partial}{\partial I^i}$
commutation and uncertainty relations	$[\hat{q}^j, \hat{p}_i] = i\hbar \delta_i^j$ $\Delta q^i \Delta p_i \geq \hbar/2$	$[\hat{I}^j, \hat{\eta}_i] = \delta_i^j k_B$ $\Delta I^i \Delta \eta_i \geq k_B$
deterministic theory	classical mechanics	thermodynamics

Table 2. Comparison between quantum mechanics and classical statistical mechanics. Despite their different mathematical structures and physical relevance, these theories exhibit several analogies as consequence of their statistical nature.

treatment for systems with a large number N of degrees of freedom, or equivalently the limit $k_B \rightarrow 0$. It is always claimed that quantum mechanics occupies an unusual place among physical theories: classical mechanics is contained as a limiting case, yet at the same time it requires this limit for its own formulation. However, it is easy to realize that this is not a unique feature of quantum mechanics. In fact, classical statistical mechanics also contains thermodynamics as a limiting case. Moreover, classical statistical mechanics requires thermodynamic notions for its own formulation, which is particularly evident in classical fluctuation theory. The interpretation of the generalized differential forces, $\eta(I|\theta) = -k_B \partial_I \log \rho(I|\theta)$, as the difference between the generalized forces ζ_i and ζ_i^m of the measuring instrument and the system shown in equation (86) is precisely based on the correspondence of classical statistical mechanics with thermodynamics through Einstein's postulate (84).

Analogously, both statistical theories demand the presence of a second system with a well-defined *deterministic description*. Any measuring instrument to study quantum mechanics is just a system that obeys classical mechanics with a sufficient accuracy, e.g.: a photographic plate. Analogously, a measuring instrument in classical statistical mechanics is a system that exhibits an accurate thermodynamical description, e.g.: a thermometer should exhibit a well-defined temperature dependence of its *thermometric variable*. If the systems under study are sufficiently small, any direct measurement involves an uncontrollable perturbation of their initial state. In particular, any experimental setup aimed to determine temperature T must involve an energy interchange via a thermal contact, which affects the internal energy E .

Conversely, it is necessary *energetic isolation* to preserve the internal energy E , thus excluding a direct determination of its temperature T .

While the classical statistical mechanics is probability theory that deals with quantities with a real character, the quantum mechanics is formulated in terms of *complex probability amplitudes* that obey the superposition principle. Despite this obvious difference, both statistical theories admit the correspondence of the physical observables with certain *operators*. Determination of the energy E and the momentum \mathbf{p} demands repeated measurements in a finite region of the space-time sufficient for observing the wave properties of the function $\Psi(\mathbf{q}, t)$. The system temperature determination also demands the exploration of a finite energy region sufficient for determining the probability density $\rho(I|\theta)$. Mathematically, these experimental procedures can be associated with differential operators: the quantum operators $\hat{E} = i\hbar\partial_t$, $\hat{\mathbf{p}} = -i\hbar\nabla$ and the statistical mechanics operator $\hat{\eta} = -k_B\partial_I$. It is easy to realize that the complementary character between the macroscopic observables I^i and the generalized differential forces η_i can be related to the fact that their respective operators $\hat{I}^i = I^i$ and $\hat{\eta}_i = -k_B\partial_{I^i}$ do not commute $[\hat{I}^i, \hat{\eta}_i] = k_B$:

$$\int_{\mathcal{M}_\theta} [\hat{I}^i, \hat{\eta}_i] \rho(I|\theta) dI \equiv \int_{\mathcal{M}_\theta} \hat{I}^i \hat{\eta}_i \rho(I|\theta) dI = k_B \Rightarrow \langle \delta I^i \delta \eta_i \rangle = k_B \Rightarrow \Delta I^i \Delta \eta_i \geq k_B. \quad (94)$$

There exist other differences between these statistical theories. For example, variables and functions describing the measuring instruments explicitly appear in probability description of classical statistical mechanics; e.g.: the entropy contribution of the measuring instrument $S^m(I|\theta)$ and the generalized forces ζ_i^m . Conversely, the measuring instruments do not appear in this explicit way in the formalism of quantum mechanics. The nature of the measuring instruments are specified in the concrete representation of the wave function Ψ . For example, the quantity $|\Psi(\mathbf{q}, t)|^2$ written in the coordinate-representation measures the probability density to detect a microparticle at the position \mathbf{q} using an appropriate measuring instrument to obtain this quantity. Analogously, the quantity $|\Psi(\mathbf{p}, t)|^2$ expressed in the momentum-representation describes the probability density to detect a particle with momentum \mathbf{p} using an appropriate *instrument* that measures a *recoil effect*.

5. Final remarks

Classical statistical mechanics and quantum theory are two formulations with different mathematical structure and physical relevance. However, these physical theories are hallmarked by the existence of *uncertainty relations between conjugated quantities*. Relevant examples are the coordinate-momentum uncertainty $\Delta q \Delta p \geq \hbar/2$ and the energy-temperature uncertainty $\Delta E \Delta(1/T - 1/T^m) \geq k_B$. According to the arguments discussed along this chapter, *complementarity* has appeared as an unavoidable consequence of the statistical apparatus of a given physical theory. Remarkably, classical statistical mechanics and quantum mechanics shared many analogies with regards to their conceptual features: (1) Both statistical theories need the correspondence with a *deterministic theory* for their own formulation, namely, classical mechanics and thermodynamics; (2) The measuring instruments play a role in the existence of complementary quantities; (3) Finally, physical observables admit the correspondence with appropriate operators, where the existence of complementary quantities can be related to their noncommutative character.

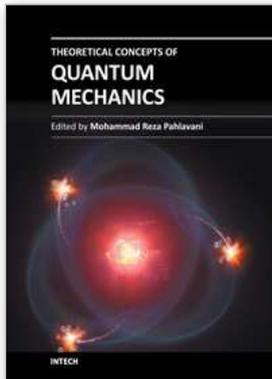
As an open problem, it is worth remarking that the present comparison between classical statistical mechanics and quantum mechanics is still uncomplete. Although the analysis

of complementarity has been focused in those systems in thermodynamic equilibrium, the operational interpretation discussed in this chapter strongly suggests the existence of a counterpart of Schrödinger equation (42) in classical statistical mechanics. In principle, this counterpart dynamics should describe the system evolutions towards the thermodynamic equilibrium, a statistical theory where Einstein's postulate (84) appears as a *correspondence principle* in the thermodynamic limit $k_B \rightarrow 0$.

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