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ON THE SEMICLASSICAL LIMIT OF EMERGENT QUANTUM MECHANICS AS
A CLASSICAL THERMODYNAMICS OF IRREVERSIBLE PROCESSES IN THE
LINEAR REGIME

DOCTORAL THESIS

BY

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ACERCA DEL LÍMITE SEMICLÁSICO DE LA MECÁNICA CUÁNTICA
EMERGENTE, COMO UNA TERMODINÁMICA CLÁSICA DE LOS PROCESOS
IRREVERSIBLES EN EL RÉGIMEN LINEAL

POR

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Abstract

Motivated by the conceptual problems concerning the quantisation of gravity, the Dutch theoretical physicist G. 't Hooft (1999 Nobel prize in physics) put forward the notion that quantum mechanics must be the emergent theory of some underlying, deterministic theory. This proposal usually goes by the name *quantum mechanics as an emergent phenomenon*. This research line, initiated by 't Hooft in the late 1990's, has been the subject of intense research over the last 15 years, by 't Hooft himself as well as by many other researchers. In this PhD thesis we present our own approach to quantum mechanics as an emergent phenomenon.

According to the emergence paradigm for quantum mechanics, information-loss effects in the underlying deterministic theory lead to the arrangement of states of the latter into equivalence classes, that one identifies as quantum states of the emergent quantum mechanics. In brief, *quantisation is dissipation*, according to 't Hooft.

Moreover it has been argued in the literature that, in the presence of weak gravitational fields, quantum effects must be indistinguishable from thermal effects. Since the latter are typically dissipative in nature, the presence of a weak gravitational field should provide a framework in which quantum effects can be explained as due to thermal, dissipative fluctuations. Furthermore, since gravitational effects can be locally gauged away (thanks to the equivalence principle), there should exist some kind of equivalence principle for quantum effects, *i.e.*, some kind of relativity principle for the notion of *quantumness* as opposed to the notion of *classicality*. In this PhD thesis we elaborate on this idea.

Once a reference frame is fixed, however, quantum effects cannot be gauged away, and the statement *quantisation is dissipation* lends itself to a thermodynamical treatment. In this thesis we also present one mechanism whereby quantum mechanics is seen to emerge, thus explicitly realising 't Hooft's proposal. This mechanism is based on a dictionary between semiclassical quantum mechanics, on the one hand, and the classical theory of irreversible thermodynamics in the linear regime, on the other. This thermodynamical formalism, developed by Nobel prize winners Onsager and Prigogine, can be easily mapped into that of semiclassical quantum mechanics.

Resumen

Motivado por los problemas conceptuales relativos a la cuantización de la gravedad, el físico teórico holandés G. 't Hooft (premio Nobel de física en 1999) sugirió la noción de que la mecánica cuántica pudiera ser la teoría emergente de alguna otra teoría determinista subyacente. Dicha propuesta se conoce como *la mecánica cuántica en tanto que teoría emergente*. Esta línea de investigación, iniciada por 't Hooft a finales de los años 90, ha sido objeto de intenso estudio a lo largo de los últimos 15 años, tanto por el mismo 't Hooft como por numerosos otros investigadores. En esta tesis doctoral presentamos nuestra propia aproximación a la mecánica cuántica como fenómeno emergente.

De acuerdo con este paradigma emergente para la mecánica cuántica, son efectos de pérdida de información en la teoría determinista subyacente los que conducen a que los estados de ésta última se agrupen en clases de equivalencia, las cuales clases se identifican con los estados cuánticos de la mecánica cuántica emergente. En breve, *la cuantización es disipación*, según 't Hooft.

Asimismo se ha argumentado en la literatura que, en presencia de campos gravitatorios débiles, los efectos cuánticos son indistinguibles de los efectos térmicos. Dado que éstos últimos son típicamente disipativos por naturaleza, la presencia de un campo gravitatorio débil debería proporcionar un entorno en el cual los efectos cuánticos puedan entenderse como debidos a fluctuaciones térmicas, disipativas. Además, dado que los campos gravitatorios pueden eliminarse localmente (gracias al principio de equivalencia), debería existir algún tipo de principio de equivalencia para los efectos cuánticos, *i.e.*, algún tipo de principio de relatividad para la noción de *cuanticidad*, por oposición a la noción de *clasicidad*. En esta tesis doctoral elaboramos estas ideas.

Sin embargo, una vez fijado un sistema de referencia, los efectos gravitatorios ya no pueden eliminarse, y la afirmación de que *la cuantización es disipación* se presta a un tratamiento termodinámico. En esta tesis también presentamos un mecanismo mediante el cual la mecánica cuántica se ve emerger, comprobándose así explícitamente la propuesta de 't Hooft. Este mecanismo se basa en un diccionario entre la mecánica cuántica semiclásica, por un lado, y la teoría clásica de la termodinámica irreversible en el régimen lineal, por otro lado. Dicho formalismo termodinámico, desarrollado por los premios Nobel Onsager y Prigogine, puede trasladarse fácilmente a la mecánica cuántica semiclásica.

Resum

Motivat pels problemes conceptuals en relació a la quantització de la gravetat, el físic teòric holandès G. 't Hooft (premi Nobel de física en 1999) va suggerir la noció de que la mecànica quàntica pogués ser la teoria emergent d' alguna altra teoria determinista subjacent. Aquesta proposta es coneix com a *mecànica quàntica en tant que teoria emergent*. Aquesta línia d'investigació, iniciada per 't Hooft a finals dels anys 90, ha sigut intensament estudiada durant els últims 15 anys, tant pel mateix 't Hooft com per nombrosos altres investigadors. En aquesta tesi doctoral presentem la nostra pròpia aproximació a la mecànica quàntica com a fenomen emergent.

D'acord amb aquest paradigma emergent per a la mecànica quàntica, són efectes de pèrdua d'informació en la teoria determinista subjacent els que condueixen a que els estats d'aquesta última s'agrupen en classes d'equivalència, les quals s'identifiquen amb els estats quàntics de la mecànica quàntica emergent. Breument, *la quantització és dissipació*, segons 't Hooft.

Així mateix, s'ha argumentat a la literatura que, en presència de camps gravitatoris febles, els efectes quàntics són indistingibles dels efectes tèrmics. Com aquests últims són típicament dissipatius per naturalesa, la presència d'un camp gravitatori feble hauria de proporcionar un entorn en el qual els efectes quàntics es puguen entendre com deguts a fluctuacions tèrmiques, dissipatives. A més a més, com que els camps gravitatoris poden eliminar-se localment (gràcies al principi d'equivalència), hauria d'existir algun tipus de principi d'equivalència per als efectes quàntics, *i.e.*, algun tipus de principi de relativitat per a la noció de *quanticitat*, per oposició a la noció de *classicitat*. En aquesta tesi doctoral elaborem aquestes idees.

En canvi, una vegada fixat el sistema de referència, els efectes gravitatoris ja no poden eliminar-se, i l'afirmació de que *la quantització és dissipació* es presta a un tractament termodinàmic. En aquesta tesi també presentem un mecanisme mitjançant el qual la mecànica quàntica es veu emergir, comprovant-se explícitament la proposta de 't Hooft. Aquest mecanisme es basa en un diccionari entre la mecànica quàntica semiclàssica, d'una banda, i la teoria clàssica de la termodinàmica irreversible en el règim lineal, d'una altra banda. Aquest formalisme termodinàmic, desenvolupat pels premis Nobel Onsager i Prigogine, pot traslladar-se fàcilment a la mecànica quàntica semiclàssica.

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Chapter 1

Overview

The two basic pillars on which modern theoretical physics stands are quantum theory and general relativity. These two theories were developed in the first quarter of the 20th century. General relativity accounts for the gravitational force, while quantum theory underlies the standard model of elementary particles.

1.1 A sketch of general relativity

According to Einstein's theory of general relativity, the gravitational force is a manifestation of the curvature of spacetime. An intuitive visualisation of this geometric approach to gravity is given by the following analogy, frequently found in popular-science books. Imagine a tablecloth spanned in a frame which is held fixed in a plane parallel to the surface of Earth. Place a heavy steel ball in the middle of the tablecloth and let a marble roll on the tablecloth. The tablecloth will be curved in the vicinity of the steel ball, and the marble's path will deviate from a straight line when it comes close to it. This is a model of the solar system with the sun replaced by the steel ball, the marble playing the role of a planet, and the 2-dimensional tablecloth replacing 3-dimensional space. The marble's path is attracted towards the steel ball—not because there is a force between the marble and the steel ball, but because the geometry of the tablecloth is curved in the neighbourhood of the steel ball.

General relativity is widely accepted as our best description of the physics of the gravitational field. It has been successfully tested in countless experiments. The perihelion rotation of Mercury, the deflection of light rays by the sun, the gravitational redshift, gravitational lensing, the Big Bang and the expansion of the universe, are perhaps the most spectacular among those predictions that have been tested experimentally beyond any reasonable doubt. On a somewhat less solid experimental footing stand other predictions, such as gravitational radiation and black holes.

Two of the above predictions are particularly remarkable because of their theoretic-

cal implications. First, the prediction that the final state of massive stars is to undergo gravitational collapse behind an event horizon and form a black hole containing a singularity, leads to a severe clash with quantum theory. The prediction concerning the Big Bang is no less remarkable: there is a singularity in our past which constitutes, in some sense, a beginning to the Universe. These two predictions of general relativity amount to an admission of the breakdown of the theory itself. Indeed, the mere presence of a singularity seems to suggest that the theory has been pushed beyond its limits of applicability.

One expects the physics of such singularities to be more correctly described by some quantum version of gravity than it is by Einstein's theory alone. There are good reasons to believe that quantum effects should play a major role in explaining the true physics of black holes and of the Big Bang. The extreme conditions believed to be present at those singularities (high density, high temperature and length scales of the order of the Planck length) require the notions of quantum mechanics for their correct description.

1.2 A sketch of quantum theory

Physics before the advent of quantum mechanics is commonly referred to as *classical*. Classical physics is a deterministic theory, its predictive power being not even limited by the (necessarily finite) resolution of our experimental devices. This is so because, in classical physics, it is always possible to compensate for experimental errors, at least in principle.

Quantum mechanics, on the other hand, is constrained by Heisenberg's principle of uncertainty. The latter imposes a fundamental restriction on the accuracy to which conjugate variables can be simultaneously measured. This restriction is independent of our experimental skills and of our technological capabilities. A consequence of this essential limitation is that quantum mechanics is an indeterministic, probabilistic, theory.

In everyday life, however, events appear to be causally connected by classical, deterministic laws. The reason indeterminism is negligible on a macroscopic scale is that macroscopic bodies are composed of a huge number of quantum particles. Macroscopic bodies comprise some 10^{23} (Avogadro's number) quantum particles; on the average, their individual nondeterministic properties balance out. In technical terms we say that this large number of particles *decohere* so, macroscopically, we can only perceive a classical average which is deterministic.

These conceptual foundations of quantum mechanics have been the subject of heated dispute ever since the early 1930's, as the so-called Copenhagen interpretation was challenged by a few but very vocal (and very remarkable) physicists, Einstein being one of them. At stake was not the predictive power of the new theory (something everybody acknowledged without reservations) but, rather, its philosophical underpinning: *God doesn't play dice!* As time went by, the Copenhagen interpretation (as

developed mainly by Bohr, Heisenberg and Born) won the day, and Einstein seemed to lose the game. In a nutshell, Einstein accepted Copenhagen quantum mechanics as a statistical theory, but refused to accept the loss of a fundamentally deterministic, ontological character that the Copenhagen interpretation brought about. For him, Copenhagen quantum mechanics was merely an effective probabilistic description of some deeper, deterministic theory, where physical entities play an ontological role independently of observation.

As quantum mechanics became established, more domains of classical physics came to be quantised. This, in turn, made the quantum theory even more successful. A well-known example of the experimental success of quantum theory is the recent discovery of the Higgs particle. Classical Yang–Mills theory can be consistently quantised because, among other things, there is a systematic procedure for getting rid of some nasty infinities that arise in the corresponding quantum theory. This procedure is called *renormalisation*—much of the credit for this goes to 't Hooft, who proved the renormalisability of (nonabelian) quantum Yang–Mills theories.

However, general relativity adamantly resisted quantisation.

1.3 Quantum mechanics meets general relativity

Severe technical difficulties arose as soon as one tried to apply the principles of quantum mechanics to the theory of relativity. Specifically, general relativity cannot be consistently quantised because it is not renormalisable. Yet one would like to have a quantum theory of gravity: a theory that describes the structure of spacetime at length scales as tiny as the Planck length. At the same time, this would-be quantum theory of gravity should be able to reproduce general relativity when considered at astronomical length scales.

This (as of yet, unsuccessful) programme has come to be known as *the quantisation of gravity*; it is an outstanding problem in 20th-century theoretical physics that penetrates deeply into the 21st century. Despite arduous efforts along many different lines of approach, a consistent theory of quantum gravity still eludes us. Those few approaches that have survived the test of time still face enormous challenges, falling short of a providing completely satisfactory solution to the problem.

To summarise: quantum mechanics and the theory of relativity have been experimentally tested innumerable times, always extremely successfully. As long as one remains within the limits of applicability of the corresponding theory, one can safely state that both theories are right. Einstein's theory of gravitation applies to the very large macroworld (*i.e.*, to astronomical scales, up to 10^{28} cm, the radius of the observable Universe). On the other hand, quantum theories describe the microworld (by which we mean length scales about the size of an atom, typically 10^{-8} cm, and below).

Gravity appears to resist all attempts to quantise it.

1.4 Quantisation—the accepted paradigm

Conceptual difficulties often require a change of mind, a change in the paradigms that underlie one's whole intellectual framework. This viewpoint is based on the conviction that any theory necessarily has certain limits, and that therefore a change in approach may be convenient, if not altogether necessary.

The quantisation of gravity is possibly one such case. The logic of the problem can be summarised as follows. One is given Einstein's *classical* theory of gravity. By *classical* one means that Planck's constant \hbar is missing: it appears nowhere in the equations. Next one applies a set of heuristic rules known as *quantisation*. These rules have been successfully applied to explain electrons, atoms, molecules, nuclei, and the whole microworld known to us, so we have some degree of confidence in them. However, they remain *a set of heuristic rules* that one applies more or less automatically, without troubling oneself much about their range of applicability.

The current paradigm in theoretical physics thus reads: *start with a classical theory, then quantise*. The resulting quantum theory is the better theory, its classical ancestor being just an approximation, sometimes a very coarse one. This paradigm has dominated much of 20th-century physics so successfully, that many physicists find it difficult to accept that there might be anything wrong with it. Perhaps the best example of the application of this paradigm is that of quantum electrodynamics, the theory of electrons and photons. In terms of explanatory power, predictive power and theoretical–numerical accuracy checked against experiments, quantum electrodynamics stands out supreme. This success story bears the names of Dirac, Feynman and Schwinger, among others. After quantum electrodynamics (an abelian Yang–Mills theory) comes the standard model of particle physics (a nonabelian Yang–Mills theory), which unifies the electromagnetic force, the weak nuclear force, and the strong nuclear force under a single principle. This second success story, also based on quantum mechanics, is associated with the names of Yang, Mills, Weinberg, Glashow and Salam, among others.

So there must be something right about the quantisation paradigm—yet, the (straightforward) quantisation of gravity turned out to be a colossal failure. Could it be the quantisation paradigm that fails?

In this PhD thesis we will analyse the possibility that the current paradigm (*start with a classical theory, then quantise*) fails for the problem at hand. It has been suggested by 't Hooft that a possible reason for this failure lies in the misconception that quantum mechanics is a *fundamental* theory. The suggestion that quantum mechanics is not a fundamental theory is elaborated throughout this PhD thesis in detail.

1.5 Emergence—a recent paradigm

So far one can state: either *general relativity is not the ultimate theory of spacetime*, or *quantum mechanics is not the ultimate theory of the microscopic world*—or both.

't Hooft takes the viewpoint that quantum mechanics as we know it, is not the ultimate theory of the microscopic world. This does not invalidate quantum mechanics as we know it. Rather, according to 't Hooft, quantum mechanics *emerges* as a probabilistic description of an *underlying* deterministic theory. In this sense, 't Hooft's view agrees with Einstein's—but one still has to actually construct such a deterministic theory in the first place, and then describe how quantum mechanics emerges from it. Einstein fell short of achieving these two goals in his critique of the Copenhagen interpretation, while 't Hooft has taken a number of ground-breaking steps towards achieving them [41, 42, 43, 44, 45, 46, 47, 48, 49, 50].

This *emergence property* of quantum mechanics is analogous to that of classical thermodynamics as derived from, say, the classical kinetic theory of gases. In the passage from the kinetic theory to the thermodynamical description there is a great deal of information loss. At a microscopic level we can, at least in principle, follow the path of each and every single molecule of gas. This entails a huge amount of information. At a macroscopic level we renounce almost all this knowledge and satisfy ourselves with just a handful of variables such as pressure, volume and temperature. Macroscopic properties can be understood and explained microscopically, but we renounce this vast amount of information. The emergent theory has entirely different properties from those of its underlying microscopic theory. Of course, classical thermodynamics is also a deterministic theory, and in this sense the analogy with quantum mechanics breaks down. However, this example serves well to illustrate the process of information loss that, according to 't Hooft, characterises the passage from an underlying deterministic theory to the probabilistic quantum mechanics that we observe and verify in our labs.

The theory underlying Copenhagen quantum mechanics, called *deterministic quantum mechanics* by 't Hooft, must first and foremost be deterministic (as opposed to probabilistic), and it must also exhibit information loss. It is a quantum theory because it describes the microscopic world, but it is deterministic because it obeys some classical equation of motion. States in the deterministic theory are arranged, by a dissipative process of information loss, into equivalence classes that the Copenhagen interpretation calls quantum states. To revert to our thermodynamical analogy, pressure can be understood as arising from the collisions of gas molecules against the container walls. Many different motions of the molecules will give rise to the same overall momentum transfer to the wall and, therefore, to the same value of the pressure. Yet, a knowledge of the pressure is far less detailed than a knowledge of the precise molecules, and the precise paths they follow as they hit the wall. So one quantum state in the Copenhagen interpretation (pressure) is the result of arranging very many different deterministic states (configurations of molecules) into one equivalence class.

Specifically, 't Hooft proves the following existence theorem: *For any quantum system there exists at least one deterministic model that reproduces all its dynamics.*

As in the previous thermodynamical analogy, the underlying deterministic theory may have little in common (at least at first sight) with the emergent statistical theory. In this way not only quantum mechanics is emergent, but possibly also its symmetries. 't Hooft further argues that symmetries we are used to such as local gauge symmetry in Yang–Mills theory, or diffeomorphism invariance in general relativity, may be emergent symmetries that need not be present, at least in their usual form, in the underlying deterministic models.

To summarise: if quantum mechanics truly is an emergent theory, then the quantisation paradigm alluded to in section 1.3 certainly breaks down, because quantum mechanics is not as fundamental as so far believed.

For completeness we would like to mention the following alternative to the statement that quantum mechanics must be an emergent phenomenon. It is usually taken for granted that the degrees of freedom of a spacetime continuum must be of a fundamental nature, *i.e.*, irreducible pieces of data, or *bits*. However, Boltzmann's dictum, *If something heats up, it has microstructure*, applies to the spacetime continuum of general relativity, because many known spacetimes can be assigned thermodynamical properties like temperature, entropy, heat capacity, etc. We do not know yet what the atoms of spacetime look like—in fact we are probably centuries away from developing the necessary technology that would allow one to probe spacetime at the Planck scale. However, the granularity of spacetime is a commonly accepted feature today, a feature that becomes invisible at the energies currently available, thus causing the impression of a continuum. In other words, spacetime might be an emergent phenomenon, too, as much as quantum mechanics.

The point of view that the spacetime continuum is a *thermodynamical* average over some (as yet unknown) atoms has been pioneered in recent years by Padmanabhan. Although we will not follow Padmanabhan's approach here, we believe it is worth mentioning in our context of emergent quantum mechanics. Indeed, there exist conceptual similarities in regarding a supposedly fundamental theory (quantum mechanics in our case, relativity in Padmanabhan's) as an effective, thermodynamical model. We have drawn fruitful inspiration from a reading of Padmanabhan's beautiful papers [58, 67, 68, 69, 70, 71, 72]. Last but not least, we would also like to mention Verlinde's influential paper [92] on the entropic character of the gravitational force as another source of inspiration for our own work.

1.6 Structure of this PhD thesis

This PhD thesis can be regarded as a natural continuation of the work begun in ref. [1]. In the latter, also a PhD thesis defended at Universidad Politécnica de Valencia under the supervision of the two current advisors, two mechanisms were presented whereby

quantum mechanics was explicitly seen to emerge, thus explicitly realising 't Hooft's proposal.

Further analysing some of the ideas put forward in ref. [1] gave rise to the present PhD thesis, which is based on the three published papers [29, 30, 31]. The publications [30] and [31] are original research articles written as part of this PhD thesis. The paper [29] contains a written version of the invited talk presented by J.M.I. at the *Sixth International Workshop DICE2012: Spacetime -Matter - Quantum Mechanics, from the Planck Scale to Emergent Phenomena*, Castiglioncello, Italy, Sept. 17-21, 2012. The material therein was already partially presented and used in ref. [1].

The contents of chapter 1 of this thesis, being a general introduction, can be found in many good expository articles and books on the subject; we claim no originality regarding this chapter. For the same reason we hardly provide bibliographic references within this chapter, since sources here are well known and easily accessible. Let us merely state that here we have, to some extent, followed the introductory chapter of ref. [1].

Chapter 2 contains a copy the article [29], which serves to set the scene and the notations for the rest of the thesis. In chapter 3 there follows a copy of the article [30]. Next, chapter 4 contains a copy of the article [31]. Finally chapter 5 presents a brief summary of our PhD thesis.

In order to respect, as closely as possible, the original text of the articles [29, 30, 31] that make up this thesis, we decided to edit the source files of each article only minimally. This has the unavoidable consequence that there may be some overlap, especially between the contents of the corresponding introductions (sections 2.1, 3.1 and 4.1). For the same reason of minimal editing, some of the equations may appear repeated throughout different chapters within the text—but never more than twice. It should be remembered, however, that each one of those articles was individually intended as a publication in its own right, as selfcontained as possible.

This minimal editing was limited to the following points:

- i)* Repetitions in the bibliography were eliminated, since all references are listed together at the end of the thesis;
- ii)* The final sections of each chapter (sections 2.5, 3.4 and 4.4) have been renamed, with respect to their counterparts in the corresponding articles, as “Conclusions to chapter 2”, “Conclusions to chapter 3” and “Conclusions to chapter 4”, respectively;
- iii)* The abstracts of the individual papers [29, 30, 31] appear collected in chapter 5, instead of being presented at the beginning of each chapter.

Bearing all of this in mind, the introductory chapter 1 thus provides the common thread that will allow the reader to navigate through the different chapters of this thesis.

Chapter 2

Emergence from irreversibility

This chapter is based on the article *Emergence from Irreversibility*, by P. Fernández de Córdoba, J.M. Isidro and Milton H. Perea, published in J. Phys. Conf. Ser. **442** (2013) 012033, available electronically as `arXiv:1210.7785 [math-ph]`, and quoted in the bibliography as ref. [29]. As compared with the original article [29], only those minor rearrangements of the material have been made that were explained in section 1.6.

2.1 Introduction

The aim of this chapter is to establish a correspondence between quantum mechanics, on the one hand, and the classical thermodynamics of irreversible processes, on the other. This we do in order to provide an independent proof of the statement that *quantum mechanics is an emergent phenomenon*.

Under the notion of an *emergent phenomenon* one usually understands the result of coarse-graining, or averaging over some deeper-level structures. These finer degrees of freedom, sometimes also called *microscopic* in order to distinguish them from the *emergent* degrees of freedom, usually carry information in such a way that they can be grouped together into higher structures, no longer microscopic, that give rise to the emergent phenomena observed in macroscopic experiments. In coarse graining microscopic information into higher structures, one is renouncing a detailed knowledge at a deeper level, in favour of some less-detailed averages, which are usually more tractable data. The canonical example of an emergent theory is classical thermodynamics, because it makes absolutely no assumption at all regarding the microscopics of the models it applies to. The corresponding microscopic theory is statistical mechanics, out of which thermodynamics emerges.

That quantum mechanics qualifies as an emergent theory has been suspected for some time [41, 44, 46, 47, 48]. In fact this topic has been the subject of a vast literature in recent years; a very incomplete list of refs. would include [13, 21, 23, 24, 25, 54,

55, 84, 87, 95]. The importance of the link between quantisation and dissipation has been explained in [10, 11, 7, 8, 9]. Some of the authors' previous work on this subject is collected in refs. [1, 2, 3, 4].

In this work we draw on the fundamental link between quantum and dissipative phenomena. By exhibiting a 1-to-1 map between quantum mechanics and the *classical* thermodynamics of *irreversible* processes, the emergent nature of quantum mechanics is laid bare. Especially relevant here are the *classical* and the *irreversible* properties of the thermodynamics involved. “Classical” means absence of \hbar ; “irreversible” implies entropy production. As will be seen below, these two facts have a clear counterpart in the quantum–mechanical description.

In section 2.2 we review some background information on the classical thermodynamics of irreversible processes. This is necessary to establish the announced correspondence, which is presented in section 2.3. The implications of this correspondence for the quantum theory are examined in section 2.4. The discussion in section 2.5 rounds up our presentation with some suggestions for future work.

2.2 Basics in irreversible thermodynamics

We first summarise, for later use, some basic elements of the classical thermodynamics of irreversible processes in the linear regime [66, 76].

Let a thermodynamical system be given, deviating only slightly from equilibrium. Assume that its entropy S depends on N extensive variables y^1, \dots, y^N , so we can write $S = S(y^1, \dots, y^N)$. The tendency of the system to seek equilibrium is measured by the *thermodynamic forces* Y_k , defined to be the components of the gradient of the entropy:

$$Y_k := \frac{\partial S}{\partial y^k}. \quad (2.1)$$

Now our system is away from equilibrium, but not too far away, so we can assume linearity between the fluxes \dot{y}^k and the forces Y_j :

$$\dot{y}^i := \frac{dy^i}{d\tau} = \sum_{j=1}^N L^{ij} Y_j, \quad Y_i = \sum_{j=1}^N R_{ij} \dot{y}^j, \quad R_{ij} = (L^{ij})^{-1}. \quad (2.2)$$

We use τ to denote thermodynamical time, and we suppose the above relation between forces and fluxes to be invertible. A well-known result is Onsager's reciprocity theorem: the matrix L is symmetric,

$$L^{ij} = L^{ji}. \quad (2.3)$$

By (2.2), the rate of entropy production can be written either as a quadratic form in the fluxes, or as a quadratic form in the forces:

$$\dot{S} = \sum_{j=1}^N \frac{\partial S}{\partial y^j} \dot{y}^j = \sum_{j=1}^N Y_j \dot{y}^j = \sum_{i,j=1}^N R_{ij} \dot{y}^i \dot{y}^j = \sum_{i,j=1}^N L^{ij} Y_i Y_j. \quad (2.4)$$

We can Taylor expand the entropy S around equilibrium and truncate the series at second order, to find

$$S = S_0 - \frac{1}{2} \sum_{i,j=1}^N s_{ij} y^i y^j + \dots, \quad (2.5)$$

where the matrix $s_{ij} = -\partial^2 S / \partial y^i \partial y^j |_0$ (the negative Hessian evaluated at equilibrium) is positive definite. This truncation has the consequence that fluctuations around equilibrium are Gaussian. Indeed, by Boltzmann's principle, the probability $P(y^1, \dots, y^N)$ of finding the values y^1, \dots, y^N of the extensive variables is given by

$$P(y^1, \dots, y^N) = Z^{-1} \exp\left(\frac{S}{k_B}\right) = Z^{-1} \exp\left(-\frac{1}{2k_B} \sum_{i,j=1}^N s_{ij} y^i y^j\right), \quad (2.6)$$

where Z is a normalisation factor.

For simplicity we set $N = 1$ in all that follows. Our aim is to calculate the probability of any path $y = y(\tau)$ in the thermodynamical configuration space. A *cumulative* distribution function $F_n \left(\begin{smallmatrix} y_1 \cdots y_n \\ \tau_1 \cdots \tau_n \end{smallmatrix} \right)$ is defined such that it yields the probability that the thermodynamical path $y(\tau)$ lie below the barriers y_1, \dots, y_n at times $\tau_1 < \tau_2 < \dots < \tau_n$:

$$F_n \left(\begin{smallmatrix} y_1 \cdots y_n \\ \tau_1 \cdots \tau_n \end{smallmatrix} \right) := P(y(\tau_k) \leq y_k, k = 1, \dots, n). \quad (2.7)$$

A stationary process is defined to be one such that F_n is invariant under time shifts $\delta\tau$:

$$F_n \left(\begin{smallmatrix} y_1 \cdots y_n \\ \tau_1 \cdots \tau_n \end{smallmatrix} \right) = F_n \left(\begin{smallmatrix} y_1 \cdots y_n \\ \tau_1 + \delta\tau \cdots \tau_n + \delta\tau \end{smallmatrix} \right). \quad (2.8)$$

In other words, the system that has been left alone long enough that any initial conditions have been forgotten. An *unconditional* probability density function $f_n \left(\begin{smallmatrix} y_1 \cdots y_n \\ \tau_1 \cdots \tau_n \end{smallmatrix} \right)$ is defined, such that the product

$$f_n \left(\begin{smallmatrix} y_1 \cdots y_n \\ \tau_1 \cdots \tau_n \end{smallmatrix} \right) dy_1 \cdots dy_n \quad (2.9)$$

measures the probability that a thermodynamical path $y = y(\tau)$ pass through a gate of width dy_k at instant τ_k , for all $k = 1, \dots, n$. Similarly, the *conditional* probability density function $f_1 \left(\begin{smallmatrix} y_k \\ \tau_k \end{smallmatrix} \middle| \begin{smallmatrix} y_{k-1} \\ \tau_{k-1} \end{smallmatrix} \right)$ is such that the product

$$f_1 \left(\begin{smallmatrix} y_k \\ \tau_k \end{smallmatrix} \middle| \begin{smallmatrix} y_{k-1} \\ \tau_{k-1} \end{smallmatrix} \right) dy_k dy_{k-1} \quad (2.10)$$

gives the probability that $y = y(\tau)$ pass through dy_k at τ_k , given that it passed through dy_{k-1} at τ_{k-1} . Finally a Markov process is defined to be *one that has a short memory* or, more precisely, one such that its cumulative, conditional probability function satisfies

$$F_1 \left(\begin{smallmatrix} y_{n+1} \\ \tau_{n+1} \end{smallmatrix} \middle| \begin{smallmatrix} y_1 \cdots y_n \\ \tau_1 \cdots \tau_n \end{smallmatrix} \right) = F_1 \left(\begin{smallmatrix} y_{n+1} \\ \tau_{n+1} \end{smallmatrix} \middle| \begin{smallmatrix} y_n \\ \tau_n \end{smallmatrix} \right). \quad (2.11)$$

One can prove that, for a Markov process, the following factorisation theorem holds [66]:

$$f_n \left(\begin{array}{c} y_1 \cdots y_n \\ \tau_1 \cdots \tau_n \end{array} \right) = f_1 \left(\begin{array}{c} y_n | y_{n-1} \\ \tau_n | \tau_{n-1} \end{array} \right) \cdots f_1 \left(\begin{array}{c} y_2 | y_1 \\ \tau_2 | \tau_1 \end{array} \right) f_1 \left(\begin{array}{c} y_1 \\ \tau_1 \end{array} \right). \quad (2.12)$$

Interesting about this factorisation theorem is the fact that $f_1 \left(\begin{array}{c} y_1 \\ \tau_1 \end{array} \right)$ is known from Boltzmann's principle. Therefore, by stationarity, all we need to know is

$$f_1 \left(\begin{array}{c} y_2 \\ \tau + \delta\tau | \tau \end{array} \right), \quad (2.13)$$

and solving the n -gate problem $f_n \left(\begin{array}{c} y_1 \cdots y_n \\ \tau_1 \cdots \tau_n \end{array} \right)$ nicely reduces to solving the 2-gate problem $f_1 \left(\begin{array}{c} y_2 \\ \tau + \delta\tau | \tau \end{array} \right)$.

Now, under the assumption that our irreversible thermodynamical processes is stationary, Markov and Gaussian, the conditional probability density (2.13) has been computed in [66], with the result

$$f_1 \left(\begin{array}{c} y_2 \\ \tau + \delta\tau | \tau \end{array} \right) = \frac{1}{\sqrt{2\pi}} \frac{s/k_B}{\sqrt{1 - e^{-2\gamma\delta\tau}}} \exp \left[-\frac{s}{2k_B} \frac{(y_2 - e^{-\gamma\delta\tau} y_1)^2}{1 - e^{-2\gamma\delta\tau}} \right]. \quad (2.14)$$

Here we have defined the thermodynamical frequency γ ,

$$\gamma := \frac{s}{R}, \quad (2.15)$$

with R given as in (2.2) and $s = -d^2 S/dy^2|_0$. Furthermore, one can reexpress the probability density (2.14) in terms of path integrals over thermodynamical configuration space: up to normalisation factors one finds [66]

$$f_1 \left(\begin{array}{c} y_2 | y_1 \\ \tau_2 | \tau_1 \end{array} \right) = \int_{y(\tau_1)=y_1}^{y(\tau_2)=y_2} Dy(\tau) \exp \left\{ -\frac{1}{2k_B} \int_{\tau_1}^{\tau_2} d\tau \mathcal{L} [\dot{y}(\tau), y(\tau)] \right\}. \quad (2.16)$$

Above we have defined the thermodynamical Lagrangian function \mathcal{L}

$$\mathcal{L} [\dot{y}(\tau), y(\tau)] := \frac{R}{2} [\dot{y}^2(\tau) + \gamma^2 y^2(\tau)], \quad (2.17)$$

whose actual dimensions are entropy per unit time.

2.3 Irreversible thermodynamics vs. quantum theory

We can now establish a precise map between quantum mechanics and classical, irreversible thermodynamics. Let t denote mechanical time, m the mass of the quantum

particle under consideration, and ω the frequency of a harmonic potential experienced by the particle.

In the first place, the thermodynamical time variable τ must be analytically continued into it :

$$\tau \leftrightarrow it. \quad (2.18)$$

Second, the thermodynamical frequency γ becomes the mechanical frequency ω of the harmonic oscillator:

$$\gamma \leftrightarrow \omega. \quad (2.19)$$

Next we map the thermodynamical variable y onto the mechanical variable x :

$$y \leftrightarrow x. \quad (2.20)$$

As a rule, x will be a position coordinate. Hence there might be some dimensional conversion factor between x and y above, that we will ignore for simplicity. Bearing this in mind, we will finally make the identification

$$\frac{s}{2k_B} \leftrightarrow \frac{m\omega}{\hbar} \quad (2.21)$$

between thermodynamical and mechanical quantities. We have expressed all the above replacements with a double arrow \leftrightarrow in order to indicate the bijective property of our map between quantum mechanics and classical, irreversible thermodynamics.

On general grounds, applying the replacements (2.18), (2.19), (2.20) and (2.21), one expects thermodynamical conditional probabilities to map onto mechanical conditional probabilities¹,

$$f_1 \left(\begin{array}{c} y_2 \\ \tau_2 \end{array} \middle| \begin{array}{c} y_1 \\ \tau_1 \end{array} \right) \leftrightarrow K(x_2, t_2 | x_1, t_1), \quad (2.22)$$

while thermodynamical unconditional probabilities are expected to map onto mechanical unconditional probabilities:

$$f_1 \left(\begin{array}{c} y \\ \tau \end{array} \right) \leftrightarrow |\psi(x, t)|^2. \quad (2.23)$$

Here $K(x_2, t_2 | x_1, t_1)$ denotes the quantum–mechanical propagator, and $\psi(x, t)$ is the wavefunction. As in (2.20) above, one must allow for possible numerical factors between probabilities on the thermodynamical and on the mechanical sides; otherwise bijectivity is perfectly preserved.

Our expectations (2.22), (2.23) are borne out by experiment—experiment in our case being explicit computation. Indeed one finds the following. For $\gamma \rightarrow 0$, the irreversible thermodynamics corresponds to the free quantum–mechanical particle:

$$K^{(\text{free})}(x_2, t | x_1, 0) = \sqrt{\frac{k_B}{s}} f_1 \left(\begin{array}{c} x_2 \\ it \\ 0 \end{array} \middle| \begin{array}{c} x_1 \\ 0 \end{array} \right)_{\gamma \rightarrow 0}, \quad (2.24)$$

¹While f_1 is a probability density, K is a probability density amplitude; see ref. [3] for a discussion of this issue.

while, for $\gamma \neq 0$, the irreversible thermodynamics corresponds to the quantum mechanics of a harmonic oscillator:

$$f_1 \left(\begin{matrix} x_2 & | & x_1 \\ it & | & 0 \end{matrix} \right) = \exp \left(\frac{i\omega t}{2} - \frac{\Delta V}{\hbar\omega} \right) \sqrt{\frac{2m\omega}{\hbar}} K^{(\text{harmonic})}(x_2, t | x_1, 0). \quad (2.25)$$

Above, $V = m\omega^2 x^2/2$ is the harmonic potential, and $\Delta V = V(x_2) - V(x_1)$. Moreover, if $\psi_0(x) = \exp(-m\omega x^2/2\hbar)$ is the harmonic oscillator groundstate, then it holds that, up to normalisation,

$$f_1 \left(\begin{matrix} x \\ it \end{matrix} \right) = \exp \left(-\frac{m\omega}{\hbar} x^2 \right) = |\psi_0^{(\text{harmonic})}(x)|^2, \quad (2.26)$$

as expected.

Finally the path–integral representation of quantum–mechanical propagators,

$$K(x_2, t_2 | x_1, t_1) = \int_{x(t_1)=x_1}^{x(t_2)=x_2} Dx(t) \exp \left\{ \frac{i}{\hbar} \int_{t_1}^{t_2} dt L[x(t), \dot{x}(t)] \right\}, \quad (2.27)$$

has a nice reexpression in terms of classical, irreversible thermodynamics. Indeed, applying our dictionary (2.18), (2.19), (2.20) and (2.21) to the mechanical path integral (2.27), the latter becomes the thermodynamical path integral already seen in (2.16). This leads us to the following relation between the action integral I of the mechanical system and the entropy S of its thermodynamical counterpart:

$$\frac{i}{\hbar} I \leftrightarrow \frac{1}{k_B} S. \quad (2.28)$$

It should be remarked that both I and S independently satisfy an extremum principle. In the Gaussian approximation considered here, the respective fluctuations (measured with respect to the corresponding mean values of I and S as given by their extremals) are obtained upon taking the exponentials. We thus obtain the quantum–mechanical wavefunction and the Boltzmann distribution function:

$$\psi = \sqrt{\rho} \exp \left(\frac{i}{\hbar} I \right), \quad \rho_B = Z^{-1} \exp \left(\frac{1}{k_B} S \right). \quad (2.29)$$

As usual, Z denotes some normalisation factor. Since, by the Born rule, we must have $\rho_B = |\psi|^2$, this provides us with an elegant expression combining thermodynamics and quantum mechanics into a single equation:

$$\psi = Z^{-1/2} \exp \left(\frac{1}{2k_B} S \right) \exp \left(\frac{i}{\hbar} I \right). \quad (2.30)$$

Eqs. (2.28) and (2.30) are very inspiring, as they reveal a fundamental complementarity between the mechanical action integral (on the mechanical side) and the entropy (on the thermodynamical side). We will later on return to the complementarity between

these two descriptions, a feature already foreseen by Prigogine [77]. For the moment let us simply remark the following consequence of this complementarity, namely, the symmetrical role played by Planck's constant \hbar and Boltzmann's constant k_B . This latter property, and the ensuing entropy quantisation, have been discussed at length in refs. [2, 3].

2.4 Emergence from irreversibility

It has been claimed that *quantisation is dissipation* [4, 10, 11, 7, 8, 9, 21, 41, 44, 84]—this claim is central to the emergence approach to quantum mechanics. In more precise terms, the previous statement implies that quantum behaviour can be expected from certain deterministic systems exhibiting information loss. One could compare this state of affairs to the relation between (equilibrium) thermodynamics and (classical) statistical mechanics. Namely, information loss in a microscopic theory (statistical mechanics) arises as the result of averaging out over many degrees of freedom; the emergent theory (thermodynamics) contains less information than its microscopic predecessor.

Thanks to the map established in section 2.3, the picture presented here features quantumness as an intrinsic property of dissipative systems. Conversely, by the same map, any quantum system features dissipation. In our picture, irreversibility and quantumness arise as the two sides of the same coin, thus becoming *complementary* descriptions of a given system (*complementarity* being understood here in Bohr's sense of the word). As opposed to the emergence property discussed above, the two theories (quantum mechanics and irreversible thermodynamics) contain exactly the same amount of information. It is interesting to observe that closely related views regarding the complementarity between mechanics and thermodynamics were defended long ago by Prigogine [77].

Now it has been (rightly) pointed out that correspondence and emergence are not quite the same concept [52]. This notwithstanding, we can still argue that quantum mechanics continues to arise as an *emergent phenomenon* in our picture. This is so because Boltzmann's dictum applies: *If something heats up, it has microstructure*. In other words, every thermodynamics is the coarse graining of some underlying statistical mechanics. Thus the mere possibility of recasting a given theory in thermodynamical language proves that the given theory is the coarse-grained version of some finer, microscopic theory.

2.5 Conclusions to chapter 2

As a technical remark, we should point out that we have worked throughout in the Gaussian approximation. On the thermodynamical side of our map this corresponds to the linear response theory; on the mechanical side this refers to the harmonic approximation. Within the regime of applicability of this assumption we can safely claim to have provided a rigorous proof of the statement that *quantum mechanics is an emergent*

phenomenon, at least in the Gaussian approximation.

Using the fact that any potential can be transformed into the free potential or into the harmonic potential by means of a suitable coordinate transformation (as in Hamilton–Jacobi theory [62, 27, 28]), one would naively state that the Gaussian approximation is good enough to “prove” that quantum mechanics is an emergent phenomenon also beyond the Gaussian regime. However, this “proof” overlooks the fact that quantisation and coordinate changes do not generally commute. Therefore the previous reasoning invoking Hamilton–Jacobi can only be seen as a plausibility argument to support the statement that quantum mechanics must remain an emergent phenomenon *also beyond* the Gaussian approximation. There is, however, abundant literature dealing with the emergent nature of quantum mechanics, *regardless of* the Gaussian approximation, using techniques that are very different from those presented here, and with a spectrum of applicability that ranges from the smallest [23, 51] to the largest [57, 75].

Chapter 3

Emergent QM as a thermal ensemble

This chapter is based on the article *Emergent Quantum Mechanics as a Thermal Ensemble*, by P. Fernández de Córdoba, J.M. Isidro and Milton H. Perea, published in *Int. J. Geom. Meth. Mod. Phys.* **11** (2014) 1450068, available electronically as [arXiv:1304.6295 \[math-ph\]](https://arxiv.org/abs/1304.6295), and quoted in the bibliography as ref. [30]. As compared with the original article [30], only those minor rearrangements of the material have been made that were explained in section 1.6.

3.1 Introduction

It has been known for long that weak interactions violate CP-invariance [16]. By the CPT theorem of quantum field theory, time invariance must also be violated in weak interactions; recent observations [61] confirm this expectation. Now quantum field theory is an extension of quantum mechanics. Since time invariance is naturally implemented in the latter, it would appear that only CP-violating quantum field theories can also violate time invariance, because quantum mechanics as we know it is symmetric under time reversal.

Actually such is not the case. A number of firmly established quantum-gravity effects have been shown to be intrinsically irreversible; for background see, *e.g.*, [41, 56, 93, 94, 97] and references therein. From the independent perspective of statistical physics [77] it has also been suggested that time irreversibility should be taken into account at the more fundamental level of the differential equations governing mechanical processes. This is in sharp contrast with standard thinking, where irreversibility is thought to arise through *time-irreversible* initial conditions imposed on the solutions to *time-reversible* evolution equations. In view of this situation, a number of authors have called for the due modifications to the standard quantum-mechanical formalism (for a detailed account and original references see, *e.g.*, [74]). Specifically, in this paper we tackle the problem of incorporating some form of time irreversibility at the level of the

differential equation governing evolution [77].

Closely related to this viewpoint is the *emergent approach* to physics. The latter has been the subject of a vast literature (see [13] for a comprehensive review), but let us briefly mention some noteworthy aspects. The notion of an *emergent theory*, that is, the concept that a given physical theory could be an effective model of some deeper-level degrees of freedom, has been postulated of a number of existing theories, most notably of gravity and of quantum mechanics. In the particular case of the latter, refs. [5, 21, 22, 40, 44, 46, 48, 88] address this issue from a number of different perspectives. The paradigm that *quantisation is dissipation*, implicitly present in some of the above approaches, has been made precise in [11, 8]. Frequently, these takes on quantum physics can be completely recast in purely classical terms [6, 54, 95]. An alternative perspective, based on classical nonequilibrium thermodynamics [66], has been advocated in [2, 4, 29]. Beyond quantum mechanics, the relevance of nonequilibrium physics for quantum gravity and strings has been emphasised recently [36, 52].

The basic physical assumption we will make use of posits that *spacetime is not a fundamental concept, but rather an emergent phenomenon instead*. In fact this hypothesis is not at all new (for references and background see, *e.g.*, [56]), some of its most recent incarnations being [67, 68, 92]. Once spacetime is no longer regarded as a fundamental concept, but rather as a derived notion, then every theory that makes use of spacetime concepts automatically qualifies as emergent. Such is the case of quantum mechanics. For our purposes it will suffice to concentrate on the time variable and expose its emergent nature. We will therefore try to express time in terms of thermodynamical quantities, and explore the consequences for the quantum theory. Again, the notion of time as having a thermodynamical origin is not new [12, 17], having reappeared more recently in [37, 78, 81, 80]; see also [20, 35, 38, 39] for related views. New to our approach is the notion that *an emergent time variable automatically implies that quantum theory itself qualifies as an emergent phenomenon*. Specifically, the possibility of reexpressing the nonrelativistic Schroedinger equation in purely entropic terms (instead of its usual Hamiltonian language) implies that quantum mechanics involves some degree of coarse graining of microscopic information. In our approach, the very existence of an entropy operator replacing the Hamiltonian operator is an unequivocal clue of this coarse graining.

To begin with, we would like to draw attention to the following analogy. On one hand we have the quantum-mechanical time-energy uncertainty relation

$$\Delta E \Delta t \gtrsim \hbar. \quad (3.1)$$

On the other hand, in the theory of irreversible thermodynamics [65, 66], one computes the average product of the fluctuations of the entropy and the temperature for a thermodynamical system slightly away from equilibrium (this is the linear regime, also called the Gaussian approximation). This product turns out to be given by [59]

$$\Delta S \Delta T = k_B T, \quad (3.2)$$

k_B being Boltzmann's constant. The change of variables

$$\tau := \ln \left(\frac{T}{T_0} \right), \quad (3.3)$$

where T_0 is some reference temperature, reduces (3.2) to

$$\Delta S \Delta \tau \gtrsim k_B. \quad (3.4)$$

In (3.4) we have taken the liberty of replacing the equality sign of (3.2) with an inequality; the latter is saturated in the Gaussian approximation (used in the derivation of (3.2)). Beyond the Gaussian regime, one expects the inequality to hold strictly. As we will see, the analogy between (3.1) and (3.4) is more than just a happy coincidence—it is in fact anything but accidental.

3.2 Emergent time

Let t and T respectively denote nonrelativistic time and absolute temperature, as measured by an inertial observer that will be kept the same throughout. We posit that t^{-1} equals T modulo dimensional factors:

$$\frac{C}{t} = \frac{k_B}{\hbar} T. \quad (3.5)$$

Here C is a dimensionless numerical factor, whose value we will pick presently in order to suit our needs. Modulo this C , which will play a prominent role in what follows, the relation (3.5) between time and temperature was postulated long ago by de Broglie [12]. A related change of variables has been used more recently in [82].

Beyond purely dimensional grounds, there are deeper motivations for Eq. (3.5). Specifically, in [4, 29] we have established a map between quantum mechanics (in the Gaussian approximation) and the classical theory of irreversible thermodynamics (in the linear regime).¹ In this latter theory [66] we have N independent thermodynamical coordinates y^1, \dots, y^N on which the entropy S depends, and N conjugate forces $Y_k := \partial S / \partial y^k$. Let t' denote thermodynamical time. The assumption of linearity between the velocities \dot{y}^k and the forces Y_j amounts to

$$\dot{y}^i = \frac{dy^i}{dt'} = \sum_{j=1}^N L^{ij} Y_j, \quad Y_i = \sum_{j=1}^N R_{ij} \dot{y}^j, \quad R_{ij} = (L^{ij})^{-1}. \quad (3.6)$$

Under the assumption that the underlying microscopic dynamics is time-reversible, the constant matrix L_{ij} turns out to be symmetric (Onsager's reciprocity theorem) [65]. By (3.6), the time rate of entropy production can be written either as a quadratic form in the velocities, or as a quadratic form in the forces:

$$\dot{S} = \sum_{i,j=1}^N R_{ij} \dot{y}^i \dot{y}^j = \sum_{i,j=1}^N L^{ij} Y_i Y_j. \quad (3.7)$$

¹As argued in [4, 29], the linear regime in irreversible thermodynamics is the analogue of the semiclassical, or Gaussian, approximation to quantum mechanics.

We see that it is not the entropy S , but its time rate of production \dot{S} , that plays the role of a (harmonic) Hamiltonian, because²

$$\dot{S} = \frac{dS}{dt'} = \frac{1}{2} \sum_{i,j=1}^N (R_{ij} \dot{y}^i \dot{y}^j + L^{ij} Y_i Y_j). \quad (3.8)$$

Here again we see that inverse time can be regarded as temperature. In Eqs. (3.6)–(3.8) above, the thermodynamical time t' and the mechanical time t are related as per the Wick rotation, $t' = it$ [4, 29]. Thus we expect a thermodynamical approach to quantum mechanics to involve the complexification of time. Multiplying (3.5) through by H/T , one realises that (3.5) is roughly equivalent to

$$C \frac{dS}{dt} = \frac{k_B}{\hbar} H, \quad (3.9)$$

which bridges the gap between the mechanical point of view (the right-hand side of (3.9)) and the thermodynamical point of view (the left-hand side). The above is a handwaving argument to justify equating the time variation of the entropy with the energy (modulo dimensional constants); we will actually *derive* Eq. (3.9) later on (see (3.26)). Eq. (3.9) is also important because it holds beyond its Gaussian limit given in (3.8). In what follows we will work out in detail the relationship between the mechanical and the thermodynamical points of view expressed above.

3.3 Entropy vs. energy

3.3.1 The energy picture

For reasons that will become apparent presently let us call quantum mechanics, in its standard formulation, the *energy picture* of quantum mechanics; we will also use the term *H-picture*.³ The evolution of pure quantum states is governed by the Schroedinger equation,

$$i\hbar \frac{d\psi}{dt} = H\psi. \quad (3.10)$$

The general solution to the above reads $\psi(t) = \mathcal{U}(t)\psi(0)$, where

$$\mathcal{U}(t) := \mathcal{T} \exp \left(-\frac{i}{\hbar} \int_0^t H(\tilde{t}) d\tilde{t} \right), \quad (3.11)$$

and \mathcal{T} denotes the ordering operation along the evolution parameter \tilde{t} . When $t \in \mathbb{R}$, the time-evolution operators $\mathcal{U}(t)$ define a 1-parameter group of unitary operators that ensure the reversibility of time flow in the *H-picture*.

² L^{ij} is positive definite for a dissipative process, hence also R_{ij} .

³We use the term *picture* instead of its synonym *representation* in order to avoid confusion with the technical meaning of the latter term in quantum-mechanical contexts such as *choice of basis in Hilbert space*, or *group representation*, or similar. Expressions such as *Schroedinger picture*, or *Heisenberg picture*, or related terms used in standard quantum mechanics should also not be confused with our use of the word *picture*.

3.3.2 The entropy picture

The purpose of this section is to develop *the entropy picture* of quantum mechanics, or the *S-picture* for short.

Under the combined changes of variables (3.5) and (3.3), the evolution equation (3.10) becomes

$$-\frac{ik_B}{C} \frac{d\psi}{d\tau} = S\psi, \quad (3.12)$$

where we have defined the entropy operator S

$$S := \frac{H}{T}. \quad (3.13)$$

The new evolution parameter τ is dimensionless, while S carries the dimension of an entropy. Our time variable τ coincides with the thermal time of [17, 78, 81], the latter specified to the nonrelativistic limit corresponding to the Schroedinger wave equation. We will see presently that $C \in \mathbb{C}$, so our evolution variable τ will actually be a complexified (or Wick-rotated), nonrelativistic, dimensionless, thermal-time variable.

The solution to the evolution equation (3.12) can be written as

$$\psi(\tau) = \mathcal{S}_C(\tau)\psi(0), \quad \tau \geq 0, \quad (3.14)$$

where

$$\mathcal{S}_C(\tau) := \mathcal{T} \exp \left(\frac{iC}{k_B} \int_0^\tau S(\tilde{\tau}) d\tilde{\tau} \right) \quad (3.15)$$

and \mathcal{T} denotes the ordering operation along the the evolution parameter $\tilde{\tau}$. If we now pick $C \in \mathbb{R}$, the evolution operators $\{\mathcal{S}_C(\tau), \tau \in \mathbb{R}\}$ in (3.15) form a 1-parameter group of unitary operators.

As long as C remains real, Eqs. (3.12)–(3.15) above simply restate standard quantum mechanics using the alternative set of variables (τ, S) . It is only for $C \notin \mathbb{R}$ that time evolution can become irreversible. For this purpose let us set, dropping an irrelevant real normalisation,

$$C := e^{i\varphi}, \quad \varphi \in \mathbb{R}. \quad (3.16)$$

On the complex plane, (3.16) corresponds to Wick-rotating the time axis by an angle φ . Now certain special values of φ are known to correspond to specific physical situations. For example, $\varphi = 0$ corresponds to standard quantum mechanics, while $\varphi = \pi$ implements the time reverse of $\varphi = 0$. The value $\varphi = -\pi/2$ gives a positive real argument within the exponential of (3.15); we will see in section 3.3.3 that this corresponds to the case of maximal entropy production, or maximal dissipation. Finally, the value $\varphi = \pi/2$ gives a negative real argument within the exponential of (3.15); this will turn out to correspond to the unphysical situation of maximal *antidissipation*. All other values of φ therefore correspond to intermediate situations between exactly unitary evolution (eventually, time-reversed) and maximal dissipation (eventually, antidissipation). For obvious reasons we must pick the quadrant corresponding to the

forward time direction and positive dissipation, *i.e.*, $\varphi \in [-\pi/2, 0]$. Let the dimensionless variable $x \in \mathbb{R}$ be a measure of the external gravitational field acting on the particle of mass m described by the Hamiltonian H , such that $x = 0$ describes the absence of gravitation, and $x \rightarrow \infty$ describes the case of a strong gravitational field acting on m . From what is known concerning the effects of gravitational fields on the quantum mechanics of particles we expect the phase φ to depend on x roughly as follows:

$$\varphi(x) = -\frac{\pi}{2} (1 - e^{-x}), \quad x \geq 0. \quad (3.17)$$

Indeed, for $x = 0$ we have a perfectly unitary evolution ($\varphi = 0$) as befits quantum particles in the absence of gravitation, while for strong gravitational fields ($x \rightarrow \infty$) we have $\varphi \rightarrow -\pi/2$, and unitarity gives way to dissipation. Of course, the precise profile (3.17) for the function $\varphi(x)$ is just one out of many possible, but it captures the right physical behaviour, namely, that gravitational fields induce thermal dissipative effects in the quantum theory, in such a way as to render quantum uncertainties indistinguishable from statistical fluctuations [85, 86]. In the absence of a gravitational field, any inertial observer perceives a clear-cut separation between these two types of fluctuations.

Altogether, (3.16) and (3.17) yield

$$C(x) = \exp \left[-\frac{i\pi}{2} (1 - e^{-x}) \right]. \quad (3.18)$$

For the rest of this paper we will concentrate on the limiting case of a weak gravitational field. So we have⁴

$$C(\varepsilon) \simeq 1 + i\varepsilon, \quad \varepsilon = -\frac{\pi x}{2}, \quad x \geq 0. \quad (3.19)$$

It remains to identify a dimensionless variable x that can provide a physically reasonable measure of a weak gravitational field acting on the quantum particle.⁵ It is standard to parametrise such a field by the metric $g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$, where $\eta_{\mu\nu}$ is the Minkowski metric, and $h_{\mu\nu}$ a small correction. It is also convenient to introduce the quantities $h_{\mu}^{\lambda} := \eta^{\lambda\alpha} h_{\mu\alpha}$ and $h := h_{\alpha}^{\alpha} = \eta^{\sigma\lambda} h_{\sigma\lambda}$. The linearised Einstein equations read

$$-16\pi T_{\mu}^{\nu} = \eta^{\sigma\lambda} \frac{\partial^2}{\partial x^{\sigma} \partial x^{\lambda}} \left(h_{\mu}^{\nu} - \frac{1}{2} \eta_{\mu}^{\nu} h \right), \quad (3.20)$$

and we can take $x = \langle h \rangle$ as a variable that satisfies our needs, at least in the weak field limit considered here. The angular brackets in $\langle h \rangle$ stand for the average value of the function h over the spacetime region of interest. That $\langle h \rangle$ is nonnegative follows from the fact that [89]

$$h = 4 \int \frac{[T_{\alpha}^{\alpha}]}{r} dx dy dz, \quad T_{\alpha}^{\alpha} \geq 0. \quad (3.21)$$

The square brackets around the trace T_{α}^{α} stand for the evaluation at a time earlier than that of interest by the interval needed for a signal to pass with unit velocity from the

⁴We will henceforth drop terms of order ε^2 and higher.

⁵In a sense, the situation analysed here is complementary to that described in ref. [53].

element $dx dy dz$ to a point a distance r apart.

Substitution of (3.19) into (3.15) leads to

$$\mathcal{S}_{1+i\varepsilon}(\tau) := \mathcal{T} \exp \left(\frac{i - \varepsilon}{k_B} \int_0^\tau S(\tilde{\tau}) d\tilde{\tau} \right), \quad (3.22)$$

and the set $\{\mathcal{S}_{1+i\varepsilon}(\tau), \tau \geq 0\}$ forms a 1-parameter *semigroup* of nonunitary operators. In the limit $\varepsilon = 0$, the set $\{\mathcal{S}_1(\tau), \tau \in \mathbb{R}\}$ becomes again the 1-parameter group of unitary operators given in (3.15) (with $C = 1$). The parameter ε allows for a continuous transition between the unitary ($\varepsilon = 0$) and the nonunitary ($\varepsilon \neq 0$) regimes.

Our choice (3.19) yields in (3.12)

$$-(i + \varepsilon)k_B \frac{d\psi}{d\tau} = S\psi. \quad (3.23)$$

It makes sense to call (3.23) the *entropic Schroedinger equation*. Again, in the limit $\varepsilon = 0$ we recover a Schroedinger-like equation,

$$-ik_B \frac{d\psi}{d\tau} = S\psi. \quad (3.24)$$

The ε term on the left-hand side of (3.23) can be regarded as a perturbative correction to the derivative term in (3.24). We see that it breaks unitarity explicitly, already at the level of the differential equation governing evolution. The physical reason for this breakdown of unitarity is the presence of an external gravitational field, the strength of which is parametrised by ε .

Altogether, Eqs. (3.22) and (3.23) define the S -picture of quantum mechanics.

3.3.3 S rather than H

One might argue that there is no need for the S -picture because the H -picture suffices. Indeed it has been known for long that a simple, “phenomenological” implementation of nonunitarity within the H -picture consists in the addition of a nonvanishing imaginary part to the time variable t in (3.10):

$$(i + \varepsilon')\hbar \frac{d\psi}{dt} = H\psi. \quad (3.25)$$

Here $\varepsilon' \in \mathbb{R}$ is a small (dimensionless) perturbation. What distinguishes (3.25) from its entropic partner (3.23), and why is the latter to be preferred over the former?

In terms of the variables (t, H) , invariance under translations in t is reflected in the conservation of the Noether charge H . There exists no preferred origin $t = 0$ for time. While (3.25) certainly leads to energy dissipation, the natural physical quantity to describe dissipation is the entropy, where one expects to find $dS/dt \geq 0$ instead of a

conservation law. In the variables (τ, S) of (3.23), one expects to have no conservation law at all; one actually finds⁶

$$\frac{dS}{dt} = \frac{k_B}{\hbar}(1 - i\varepsilon)H, \quad (3.26)$$

as anticipated in (3.9). Now, from (3.8) and the Wick rotation $t' = it$, we conclude that it is $\text{Im}(dS/dt)$, and not $\text{Re}(dS/dt)$, that accounts for dissipation. Indeed, recalling (3.5), the real part of (3.26) is the usual thermodynamical definition of temperature, $\partial S/\partial E = 1/T$. In other words, even if $\text{Re}(dS/dt) = k_B H/\hbar \neq 0$, this latter equation alone does not account for dissipation. Since

$$\text{Im}\left(\frac{dS}{dt}\right) = -\varepsilon \frac{k_B}{\hbar}H, \quad (3.27)$$

there will be no conservation law for S under evolution in t if $\varepsilon \neq 0$. The same conclusion applies to evolution in τ . Furthermore, dissipation vanishes in the limit $\varepsilon = 0$ as had to be the case. Finally, for Eq. (3.27) to be consistent with the second law of thermodynamics, we need to choose $\varepsilon < 0$, as anticipated in (3.19). This latter point is obvious in the Gaussian approximation (3.8), where H is a positive-definite quadratic form, but it also holds true beyond that approximation, because H is bounded from below (if needed, one adds a constant to shift the energy of the groundstate, to make it nonnegative).

As already remarked, the operators (3.22) are unitary iff $\varepsilon = 0$. Here we see that their nonunitarity differs considerably in the two cases $\varepsilon > 0$ and $\varepsilon < 0$. Since $\tau \geq 0$, had ε been positive, this would have turned the $S_{1+i\varepsilon}(\tau)$ into a semigroup of *contraction operators* [96], which would describe an unphysical *antidissipative* world. On the contrary, the choice $\varepsilon < 0$ of (3.19) leads to the opposite behaviour, *dilatation*, which is in agreement with the second law of thermodynamics.

In the H -picture, whenever the Hamiltonian is time-independent, there exist energy eigenstates ϕ satisfying $H\phi = E\phi$; the wavefunction ψ then factorises as $\psi = \phi \exp(-iEt/\hbar)$. A similar property holds in the S -picture, assuming that H remains t -independent, hence also τ -independent. In this latter case one can readily check that the factorised wavefunctions

$$\psi = \phi e^{(i-\varepsilon)\tau s}, \quad (3.28)$$

where ϕ does not depend on τ , lead to the eigenvalue equation

$$S\phi = s k_B \phi, \quad (3.29)$$

with $s \in \mathbb{R}$ playing the role of a dimensionless entropic eigenvalue. Again, eqs. (3.28) and (3.29) above are in perfect agreement with the second law of thermodynamics.

To summarise, unitarity is violated in the S -picture, where $\varepsilon < 0$ appears, but not in the H -picture, where the evolution equations (3.10) and (3.11) remain strictly

⁶Here we are assuming $dH/dt = 0$ for simplicity.

valid. As such, this “change of picture” between H and S is an instance of Prigogine’s *nonunitary transformation* [77]. The apparent dilemma, “Is unitarity violated or not?”, will be resolved in section 3.3.6.

3.3.4 Uncertainty vs. the second law

It is common lore that, at least for large enough temperatures, quantum fluctuations are negligible compared to thermal statistical fluctuations [59]. When stating that, *in the presence of a gravitational field*, quantum fluctuations are inextricably linked with thermal statistical fluctuations, one is postulating a new kind of uncertainty principle: *the indistinguishability between quantum and statistical fluctuations* [14, 85, 86]. Here we will provide an example of this indistinguishability. A look at Eq. (3.1) and a comparison of (3.23) with (3.10) leads one to conclude the following uncertainty relation:

$$\Delta S \Delta \tau \gtrsim k_B. \quad (3.30)$$

It is rewarding to see the product of *thermal fluctuations* found in (3.4) nicely matched by the product of *quantum–mechanical uncertainties* (3.30). This is more than just a coincidence—it is an expression of the fact that, *in the presence of a gravitational field*, quantum uncertainties can be understood as statistical fluctuations possessing a thermal origin [85, 86]. The above uncertainty relation leads to the factor $2k_B$ replacing the quantum of action \hbar , in perfect agreement with the results of [82].

Since τ is dimensionless, we can safely set $\Delta \tau = 1$ in (3.30) with the certainty that this numerical value will not change upon changing units. This leads to

$$\Delta S \geq k_B > 0, \quad (3.31)$$

which becomes the familiar second law of thermodynamics when written as

$$\Delta S \geq 0. \quad (3.32)$$

Strictly speaking, the equality in (3.32) is never attained, as $k_B > 0$. However, in the limit $k_B \rightarrow 0$ we can saturate the inequality in (3.32) and have $\Delta S = 0$. The limit $k_B \rightarrow 0$ has been argued to correspond to the semiclassical limit $\hbar \rightarrow 0$ of quantum mechanics [2].⁷

We conclude that the quantum–mechanical uncertainty principle provides the refinement (3.31) of the second law of thermodynamics (3.32), to which it becomes strictly equivalent in the semiclassical limit $k_B \rightarrow 0$.

3.3.5 Commutators vs. fluctuations

In the standard quantum–mechanical formalism, nonvanishing commutators account for uncertainties. Fortunately for us, uncertainties can arise from fluctuations just as

⁷In order to conform to the conventions of ref. [92], in ref. [2] we have normalised the quantum of entropy to the value $2\pi k_B$ instead of the value $2k_B$ used here.

well as from commutators. In keeping with our previous arguments, here we will take statistical fluctuations as our starting point, in order to arrive at commutators.

We will illustrate our point by means of an example. Consider a thermodynamical system described by the temperature T , the pressure p , the volume V and the entropy S . Now, in the Gaussian approximation, the probability P of a fluctuation Δp , ΔV , ΔT , ΔS is given by [59]

$$P = Z^{-1} \exp \left[-\frac{1}{2k_B T} (-\Delta p \Delta V + \Delta T \Delta S) \right]. \quad (3.33)$$

If we have an equation of state $F(p, V, T) = 0$ we can solve for the temperature to obtain $T = g(p, V)$. This allows us to rewrite (3.33) as

$$P = Z^{-1} \exp \left[-\frac{1}{2k_B} \left(-\frac{\Delta p \Delta V}{g(p, V)} + \frac{\Delta T \Delta S}{T} \right) \right]. \quad (3.34)$$

This somewhat clumsy expression can be further simplified if we assume our system to be an ideal gas, $pV = S_0 T$:⁸

$$P = Z^{-1} \exp \left[-\frac{1}{2k_B} \left(-S_0 \frac{\Delta p \Delta V}{pV} + \frac{\Delta T \Delta S}{T} \right) \right]. \quad (3.35)$$

Finally define the dimensionless variables

$$p_1 := -\ln \left(\frac{p}{p_0} \right), \quad q_1 := \ln \left(\frac{V}{V_0} \right), \quad p_2 := \ln \left(\frac{T}{T_0} \right), \quad q_2 := \frac{S}{S_0}, \quad (3.36)$$

where p_0, V_0, T_0, S_0 are fixed reference values, to arrive at

$$P = Z^{-1} \exp \left[-\frac{S_0}{2k_B} (\Delta p_1 \Delta q_1 + \Delta p_2 \Delta q_2) \right]. \quad (3.37)$$

The argument of the above exponential is very suggestive. Indeed, let q_1, q_2 be coordinates on the thermodynamical configuration space Y , and consider the (dimensionless) symplectic form on the cotangent bundle T^*Y given by

$$\Omega = dp_1 \wedge dq_1 + dp_2 \wedge dq_2. \quad (3.38)$$

We have

$$\Omega = d\theta, \quad \theta := p_1 dq_1 + p_2 dq_2. \quad (3.39)$$

Now $\Delta p_1 \Delta q_1 + \Delta p_2 \Delta q_2$ equals the (symplectic) area of a 2-dimensional open surface D within T^*Y ,

$$\Delta p_1 \Delta q_1 + \Delta p_2 \Delta q_2 = \int_D (dp_1 \wedge dq_1 + dp_2 \wedge dq_2) = \int_D d\theta, \quad (3.40)$$

⁸Here S_0 is the mole number n times the gas constant R . Whether or not our system is an ideal gas is immaterial, as the change of variables (3.36) can be modified appropriately without altering our conclusions.

the boundary of which is $\partial D \neq 0$ (the surface D can be taken to be open precisely because D is caused by a fluctuation). Applying Stokes' theorem we can thus write for the probability (3.37)

$$\begin{aligned} P &= Z^{-1} \exp \left(-\frac{S_0}{2k_B} \int_D \Omega \right) \\ &= Z^{-1} \exp \left(-\frac{S_0}{2k_B} \int_D d\theta \right) = Z^{-1} \exp \left(-\frac{S_0}{2k_B} \int_{\partial D} \theta \right). \end{aligned} \quad (3.41)$$

Starting from fluctuations, which render commutators unnecessary in the thermodynamical description, we have arrived back at a mechanical description in terms of a symplectic form. The inverse of the latter gives Poisson brackets and, upon quantisation, commutators. This simple example illustrates the thermodynamical analogue of quantum commutators.

3.3.6 Quantumness vs. dissipation

To round up our presentation of quantum theory in thermodynamical terms, let us see how suggestive Eq. (3.5) is of a closely related geometric construction.

Assume being given two copies of the complex plane \mathbb{C} , one parametrised by the complex coordinate z , the other by w . Then the set formed by the two coordinate charts $\{z \in \mathbb{C}\}$ and $\{w \in \mathbb{C}\}$ defines an (analytic) atlas covering the Riemann sphere S^2 , where $z = 0$ (respectively, $w = 0$) corresponds to the north pole (respectively, south pole). The transition between these coordinates is $w = -1/z$, which coincides with (3.5) up to dimensional constants.

In this way it is very tempting to identify (t, T) with (z, w) ; of course, the latter are real 2-dimensional variables, while the former are real 1-dimensional. We may thus regard the pair “time, temperature” as coordinates on a copy of the circle S^1 that one might call *the circle of time*, or *the circle of temperature* just as well [18]. Since the circle S^1 is a compact manifold, charting it smoothly requires at least two coordinate charts (in our case T and t). In physical terms, temperature is the physical variable that compactifies time, and viceversa [63]. The rotation (by 2π radians) of any circle S^1 joining the north and south poles spans the whole sphere S^2 . This same geometrical rotation (now by an angle ε) corresponds to the Wick rotation of (3.19). Thus Wick-rotating the circle of time S^1 by all possible angles generates the whole sphere S^2 .

Now, the H -picture discussed in section 3.3.1 corresponds to viewing quantum mechanics *in the absence of dissipation*. As already observed, this situation corresponds to *the absence of a gravitational field*. On the Riemann sphere S^2 , the H -picture describes quantum mechanics with respect to an evolution parameter t that runs over the real axis $\text{Im}(z) = 0$ within the coordinate chart $\{z \in \mathbb{C}\}$ around the north pole. Dissipation appears when Wick-rotating this axis by $\varepsilon < 0$ as done in (3.19) and changing variables as per (3.5), in order to work in the coordinate chart $\{w \in \mathbb{C}\}$ around the south pole; this is how the S -picture of section 3.3.2 arises. The H -picture is purely conservative (because it satisfies the conservation law $dH/dt = 0$), the S -picture is

dissipative (because it satisfies the second law $\text{Im}(dS/dt) \geq 0$). We realise that the S -picture involves dissipation/gravity, while the H -picture involves neither. This is analogous to the equivalence principle of gravitation, whereby the action of a gravitational field can be (locally) turned off by an appropriate change of coordinates.

The foregoing arguments implement a relativity of the notion of *quantumness* vs. *dissipation* by means of $U(1)$ -transformations. However this $U(1)$ symmetry of Wick rotations is broken the very moment one selects a specific value for ε . Hence the distinction between quantumness and dissipation (falsely) appears to be absolute, while in fact it is not. In particular, just as gravity can be (locally) gauged away, so can dissipation. Turn this argument around to conclude that *quantumness, or alternatively dissipation, can be gauged away*, although never the two of them simultaneously. Quantumness is gauged away in the limit $\varphi \rightarrow -\pi/2$, while dissipation is gauged away in the limit $\varphi \rightarrow 0$.⁹ Moreover, our statement concerning the *relativity of dissipation* is equivalent to our statement concerning the *relativity of quantumness*. A concept closely related to this latter notion was put forward in [79]. Compare now the concept *relativity of quantumness* with its transpose *quantum relativity*, or *quantum gravity* as usually called: beyond the pun on words, these two concepts appear to be complementary, in Bohr's sense of the term "complementarity".

3.4 Conclusions to chapter 3

The approach to quantum mechanics presented in this chapter represents an attempt to meet the requirement (demanded *e.g.* in [75, 85, 86], among others) that gravity be incorporated into the foundations of quantum theory. The absence of a link between quantum and gravitational effects in the standard formulation of quantum theory is a feature that has been claimed to lie at the heart of some of the conceptual difficulties facing the foundations of quantum mechanics.

Specifically, in this paper we have presented a thermodynamical approach (following the classical theory of irreversible thermodynamics [65, 66, 77]) that provides a viable answer to this request, at least in a certain limit to be specified below. The incorporation of gravitational effects in a discussion of the principles of quantum mechanics is being addressed here through the appearance of dissipation as a gravitational effect. In this way the time-reversal symmetry of quantum mechanics is destroyed. Nonunitarity is implemented here by means of a Wick rotation; the latter is a consequence of gravitation. In fact Wick rotations of the time axis are the quantum-mechanical counterpart to the equivalence principle of gravitation. Just as gravity can be (locally) gauged away, so can dissipation/quantumness.

For ease of reference, below we present Eqs. (3.5), (3.22), (3.23), (3.27) and (3.30) again in order to summarise the relevant expressions of the S -picture of quantum me-

⁹Since we have systematically dropped terms of order ε^2 and higher, some of our expressions may need amendments before taking the limit $\varphi \rightarrow -\pi/2$, but this does not invalidate our reasoning.

chanics developed in this paper. We have

$$\frac{e^{i\varepsilon}}{t} = \frac{k_B}{\hbar} T, \quad \tau = \ln\left(\frac{T}{T_0}\right), \quad (3.42)$$

which relates inverse time and temperature through a Wick rotation by a small, dimensionless parameter $\varepsilon < 0$. The latter encodes the strength of an external gravitational field; in the absence of gravitation we have $\varepsilon = 0$. Applying the change of variables (3.42), the usual Schroedinger equation and the uncertainty principle become

$$k_B \frac{d\psi}{d\tau} = (i - \varepsilon) S \psi, \quad S = \frac{H}{T}, \quad \Delta S \Delta \tau \gtrsim k_B, \quad (3.43)$$

where the Hamiltonian operator H is replaced with the entropy operator S . This entropic Schrodinger equation is solved by $\psi(\tau) = \mathcal{S}(\tau)\psi(0)$, where the evolution operators $\mathcal{S}(\tau)$ in the dimensionless parameter τ , defined as

$$\mathcal{S}(\tau) := \mathcal{T} \exp\left(\frac{i - \varepsilon}{k_B} \int_0^\tau S(\tilde{\tau}) d\tilde{\tau}\right), \quad (3.44)$$

satisfy a 1-parameter semigroup of nonunitary operators (above, \mathcal{T} denotes operator ordering along the parameter $\tilde{\tau} \geq 0$). Finally the expression

$$\text{Im}\left(\frac{dS}{dt}\right) = -\varepsilon \frac{k_B}{\hbar} H \quad (3.45)$$

relates the rate of entropy production to the Hamiltonian operator, while at the same time fixing the sign of ε to be negative, in compliance with the second law of thermodynamics.

The previous equations hold in the limiting case of a weak gravitational field acting on a quantum particle described by the same equations. In view of the smallness of ε in (3.44), it is only for large values of τ that one can hope to measure the appearance of unitarity loss. It is important to realise that, by just switching back and forth between the energy picture (standard quantum mechanics) and the entropy picture (as summarised in Eqs. (3.42), (3.43), (3.44) and (3.45)), either quantumness or dissipation can be gauged away, though never the two of them simultaneously. This fact we take as a reflection of the equivalence principle of relativity, whereby gravitational fields can be (locally) gauged away by means of coordinate changes.

The postulate (3.5) (first presented long ago by de Broglie [12] without the Wick rotation $e^{i\varepsilon}$) leads to *considering time as emergent a property as temperature itself*. In this way unitarity violation can also be regarded as an emergent phenomenon.

Chapter 4

The irreversible quantum

This chapter is based on the article *The Irreversible Quantum*, by P. Fernández de Córdoba, J.M. Isidro, Milton H. Perea and J. Vazquez Molina, published in *Int. J. Geom. Meth. Mod. Phys.* **12** (2015) 1550013, available electronically as `arXiv:1311.2787 [quant-ph]`, and quoted in the bibliography as ref. [31]. As compared with the original article [31], only those minor rearrangements of the material have been made that were explained in section 1.6.

4.1 Introduction

In his Nobel Prize Lecture, Prigogine advocated an intriguing type of “complementarity between dynamics, which implies the knowledge of trajectories or wavefunctions, and thermodynamics, which implies entropy” [77]. Another Nobel Prize winner, ’t Hooft, has long argued that quantum mechanics must emerge from some underlying deterministic theory via information loss [49]. Entropy is of course intimately related to information loss, hence one expects some link to exist between these two approaches to quantum theory.

In an apparently unrelated venue, the Chapman–Kolmogorov equation [19]

$$F(z_1)F(z_2) = F(z_1 + z_2), \quad (4.1)$$

is a functional equation in the unknown F , where z_1, z_2 are any two values assumed by the complex variable z . It has the general solution

$$F_a(z) = e^{za}, \quad (4.2)$$

with $a \in \mathbb{C}$ an arbitrary constant. Implicitly assumed above is the multiplication rule for complex numbers. In other words, (4.2) solves (4.1) within a space of number-valued functions. If we allow for a more general multiplication rule such as matrix multiplication (possibly infinite-dimensional matrices), then the general solution

(4.2) of the functional equation (4.1) can be allowed to depend parametrically on a z -independent, constant *matrix* or *operator* A acting on some linear space:

$$F_A(z) = e^{zA}. \quad (4.3)$$

The functional equation (4.1), in its different guises, will play an important role in what follows. We see that its solutions are by no means unique, depending as they do on the space where one tries to solve the equation. Moreover, we will see that the question of specifying one solution space or another will bear a close relation to the question posed at the beginning—namely, the duality between thermodynamics and mechanics, on the one hand, and the emergence property of quantum mechanics, on the other.

Let \mathcal{X} and \mathcal{Y} respectively stand for the configuration spaces of a mechanical system and a thermodynamical system, the latter taken slightly away from equilibrium. We will be interested in the quantum theory based on \mathcal{X} , and in the theory of irreversible thermodynamics in the linear regime based on \mathcal{Y} [66]. There exist profound analogies between these two theories [4, 30, 64, 82, 83]. Furthermore, seeming mismatches between the two actually have a natural explanation in the context of the emergent approach to quantum theory [5, 13]; closely related topics were analysed long ago in [12] and more recently in [15, 26, 32, 33, 34, 58, 63, 73, 90, 91]. One of these mismatches concerns the irreversibility of time evolution in the thermodynamical picture, as opposed to its reversibility in the quantum–mechanical picture.

The standard quantum formalism is invariant under time reversal. This is reflected, *e.g.*, in the fact that the Hilbert space of quantum states $L^2(\mathcal{X})$ is complex and self-dual [96], so one can exchange the incoming state $|\phi\rangle$ and the outgoing state $\langle\psi|$ by Hermitean conjugation, without ever stepping outside the given Hilbert space $L^2(\mathcal{X})$. On the other hand, the thermodynamical space of states is the complex Banach space $L^1(\mathcal{Y})$ of complex-valued, integrable probability densities $\phi : \mathcal{Y} \rightarrow \mathbb{C}$. This is in sharp contrast to the square-integrable probability density *amplitudes* of quantum theory. Now the topological dual space to $L^1(\mathcal{Y})$ is the Banach space $L^\infty(\mathcal{Y})$ [96]. These two spaces fail to qualify as Hilbert spaces. In other words, for any $|\phi\rangle \in L^1(\mathcal{Y})$ and any $\langle\psi| \in L^\infty(\mathcal{Y})$,¹ the respective norms $\|\phi\|_1$ and $\|\psi\|_\infty$ are well defined, but neither of these derives from a scalar product. All there exists is a nondegenerate, bilinear pairing

$$(\cdot|\cdot) : L^\infty(\mathcal{Y}) \times L^1(\mathcal{Y}) \longrightarrow \mathbb{C} \quad (4.4)$$

taking the covector $\langle\psi|$ and the vector $|\phi\rangle$ into the number $(\psi|\phi)$:

$$(\psi|\phi) := \int_{\mathcal{Y}} \psi^* \phi. \quad (4.5)$$

Under these circumstances there is no exchanging the incoming state $|\phi\rangle \in L^1(\mathcal{Y})$ and the outgoing state $\langle\psi| \in L^\infty(\mathcal{Y})$, as they belong to different spaces. Therefore time

¹We follow the notations of ref. [4]. In particular, the round brackets in $|\phi\rangle$ and $\langle\psi|$ refer to $L^1(\mathcal{Y})$ and its topological dual $L^\infty(\mathcal{Y})$, respectively, while the angular brackets of the quantum–mechanical ket $|\phi\rangle$ and bra $\langle\psi|$ refer to $L^2(\mathcal{X})$ and its topological dual $L^2(\mathcal{X})$. Concerning the measure on \mathcal{X} and \mathcal{Y} , see below in the main text.

reversal symmetry is lost. We see that *dispensing with the scalar product in quantum theory is the same as dispensing with time reversal symmetry.*

We have in [4, 30] touched on several basic issues concerning a thermodynamical formalism for quantum theory. Specifically, a map has been constructed between the quantum mechanics of a finite number of degrees of freedom, on the one hand, and the theory of irreversible processes in the linear regime, on the other. The current paper elaborates further on the properties of a *thermodynamical dual theory* for emergent quantum mechanics. The underlying logic might be briefly summarised as follows:

- i)* it has been claimed that thermodynamics is complementary, or dual, to mechanics;
- ii)* mechanics is symmetric under time reversal while thermodynamics is not;
- iii)* dispensing with time reversal symmetry is the same as dispensing with the scalar product in quantum theory;
- iv)* the representation of the Chapman–Kolmogorov equation (4.1) on the quantum mechanical Hilbert space $L^2(\mathcal{X})$ makes decisive use of the scalar product;
- v)* here we construct representations of (4.1) on the thermodynamical Banach spaces $L^1(\mathcal{Y})$ and $L^\infty(\mathcal{Y})$, where no scalar product is present.

For simplicity we will henceforth assume \mathcal{X} and \mathcal{Y} both equal to \mathbb{R} , the latter endowed with the Lebesgue measure.

The aim of our paper is not to reformulate the theory of irreversible thermodynamics as originally developed in [66]. Rather, *we intend to exhibit irreversibility as a key property of quantum–mechanical behaviour.*

4.2 Different representations for Chapman–Kolmogorov

4.2.1 The quantum–mechanical representation

In quantum mechanics it is customary to write (4.1) as

$$U(t_1)U(t_2) = U(t_1 + t_2), \quad t \in \mathbb{R}, \quad (4.6)$$

and to call it the *group property* of time evolution. If H denotes the quantum Hamiltonian operator (assumed time–independent for simplicity), then (4.6) is solved by matrices such as (4.3), here called time–evolution operators and defined as

$$U(t) := \exp\left(-\frac{i}{\hbar}tH\right). \quad (4.7)$$

The solutions of (4.6) satisfy the differential equation

$$i\hbar \frac{dU}{dt} = HU(t), \quad H = i\hbar \left. \frac{dU}{dt} \right|_{t=0}. \quad (4.8)$$

Comparing (4.7) with (4.3) we have $z = t$ and $A = -iH/\hbar$. The $U(t)$ are unitary on $L^2(\mathbb{R})$. In a basis of position eigenfunctions $|x\rangle$, the matrix elements of $U(t)$ equal the

Feynman propagator: $\langle x_2|U(t_2 - t_1)|x_1\rangle = K(x_2, t_2|x_1, t_1)$. In terms of the latter, one rewrites the group property (4.6) as

$$K(x_3, t_3|x_1, t_1) = \int dx_2 K(x_3, t_3|x_2, t_2) K(x_2, t_2|x_1, t_1). \quad (4.9)$$

There is a path integral for the Feynman propagator K :

$$K(x_2, t_2|x_1, t_1) = \int_{x(t_1)=x_1}^{x(t_2)=x_2} Dx(t) \exp \left\{ \frac{i}{\hbar} \int_{t_1}^{t_2} dt L[x(t), \dot{x}(t)] \right\}, \quad (4.10)$$

where L is the classical Lagrangian function.

To summarise, the operators (4.7) provide a unitary representation of the commutative group (4.6) on the Hilbert space $L^2(\mathbb{R})$.

4.2.2 Intermezzo

Here we recall some technicalities to be used later; a good general reference is [96].

$L^1(\mathbb{R})$ is the space of all Lebesgue measurable, absolutely integrable functions $\phi : \mathbb{R} \rightarrow \mathbb{C}$, *i.e.*, functions such that $\int_{\mathbb{R}} |\phi(y)| dy < \infty$. This is a complex Banach space with respect to the norm $\|\psi\|_1 := \int_{\mathbb{R}} |\phi(y)| dy$.² A *denumerable* basis (a Schauder basis) exists for $L^1(\mathbb{R})$.

The topological dual space to $L^1(\mathbb{R})$ is $L^\infty(\mathbb{R})$, a duality between the two being given in Eqs. (4.4), (4.5). $L^\infty(\mathbb{R})$ is the space of all Lebesgue measurable functions $\psi : \mathbb{R} \rightarrow \mathbb{C}$ that are essentially bounded, *i.e.*, functions that remain bounded on all \mathbb{R} except possibly on a set of measure zero. $L^\infty(\mathbb{R})$ is a Banach space with respect to the norm $\|\cdot\|_\infty$, defined as follows. A nonnegative number $\alpha \in \mathbb{R}$ is said to be an essential upper bound of ψ whenever the set of points $y \in \mathbb{R}$ where $|\psi(y)| \geq \alpha$ has zero measure. The norm $\|\psi\|_\infty$ is the infimum of all those α :

$$\|\psi\|_\infty := \inf \{ \alpha \in \mathbb{R}^+ : \alpha \text{ essential upper bound of } \psi \}. \quad (4.11)$$

A key property is that one can pointwise multiply $\psi \in L^\infty(\mathbb{R})$ with $\phi \in L^1(\mathbb{R})$ to obtain $\psi\phi \in L^1(\mathbb{R})$ because $\int_{\mathbb{R}} |\psi\phi| dy < \infty$; this is used decisively in the pairing (4.5). Another key property of $L^\infty(\mathbb{R})$ is that it admits no Schauder basis.

The space $L^1(\mathbb{R})$ is canonically and isometrically embedded into its topological bidual, *i.e.*, $L^1(\mathbb{R}) \subset L^1(\mathbb{R})^{**}$. Since $L^1(\mathbb{R})$ is nonreflexive, this inclusion is strict, a property that will be used later on.³ Finally, the absence of a scalar product on $L^1(\mathbb{R})$ and $L^\infty(\mathbb{R})$ does not prevent the existence of unitary operators on them, the latter being defined as those that preserve the corresponding norm.

²Just for comparison, the norm on the Hilbert space $L^2(\mathbb{R})$ is $\|\phi\|_2 := (\int_{\mathbb{R}} |\phi(y)|^2 dy)^{1/2}$.

³The topological complementary space to $L^1(\mathbb{R})$, *i.e.*, the space Z such that $L^1(\mathbb{R})^{**} = L^1(\mathbb{R}) \oplus Z$, is known in the literature, but it will not be necessary here.

4.2.3 The representation in irreversible thermodynamics

In statistics, the Chapman–Kolmogorov equation (4.1) was well known before the advent of quantum theory [19]. Here one is given a certain measure space \mathcal{Y} (here assumed equal to \mathbb{R} endowed with the Lebesgue measure) and the corresponding Banach spaces $L^1(\mathbb{R})$ and its topological dual $L^\infty(\mathbb{R})$. These two will become carrier spaces for representations of the Chapman–Kolmogorov equation (4.1).

One calls $f_1 \left(\begin{smallmatrix} y_2 \\ \tau_2 \end{smallmatrix} \middle| \begin{smallmatrix} y_1 \\ \tau_1 \end{smallmatrix} \right)$ the *conditional* probability that the random variable $y \in \mathbb{R}$ takes on the value y_2 at time τ_2 provided that it took on the value y_1 at time τ_1 . Then one usually writes the Chapman–Kolmogorov equation (4.1) in a manner similar to (4.9),

$$f_1 \left(\begin{smallmatrix} y_3 \\ \tau_3 \end{smallmatrix} \middle| \begin{smallmatrix} y_1 \\ \tau_1 \end{smallmatrix} \right) = \int dy_2 f_1 \left(\begin{smallmatrix} y_3 \\ \tau_3 \end{smallmatrix} \middle| \begin{smallmatrix} y_2 \\ \tau_2 \end{smallmatrix} \right) f_1 \left(\begin{smallmatrix} y_2 \\ \tau_2 \end{smallmatrix} \middle| \begin{smallmatrix} y_1 \\ \tau_1 \end{smallmatrix} \right), \quad (4.12)$$

which expresses the Bayes rule for conditional probabilities. A representation of this equation by means of linear operators $\mathcal{U}(\tau)$ on $L^1(\mathbb{R})$ and on $L^\infty(\mathbb{R})$ would thus have to satisfy the algebra

$$\mathcal{U}(\tau_1)\mathcal{U}(\tau_2) = \mathcal{U}(\tau_1 + \tau_2), \quad (4.13)$$

which is again a presentation of (4.1). We can immediately read off the matrix elements of $\mathcal{U}(\tau)$:

$$\langle y_2 | \mathcal{U}(\tau_2 - \tau_1) | y_1 \rangle = f_1 \left(\begin{smallmatrix} y_2 \\ \tau_2 \end{smallmatrix} \middle| \begin{smallmatrix} y_1 \\ \tau_1 \end{smallmatrix} \right). \quad (4.14)$$

As opposed to the quantum–mechanical case, the carrier space for the representation of the algebra (4.13) is Banach but not Hilbert. The reason for this is that one deals directly with probabilities rather than amplitudes.

The question arises: if one were to express the matrix (4.14) in the form given by the general solution (4.3), then clearly one would have $z = \tau$, but what would the operator A be? It is mathematically true, though physically unsatisfactory, to claim that A would be (proportional to) the logarithm of $\mathcal{U}(\tau)$. One of the purposes of this paper is to determine the operator A explicitly, and to interpret it in the terms stated in the introduction. However, in order to do this, a knowledge of the conditional probabilities $f_1 \left(\begin{smallmatrix} y_2 \\ \tau_2 \end{smallmatrix} \middle| \begin{smallmatrix} y_1 \\ \tau_1 \end{smallmatrix} \right)$ is needed.

There are a number of instances in which the $f_1 \left(\begin{smallmatrix} y_2 \\ \tau_2 \end{smallmatrix} \middle| \begin{smallmatrix} y_1 \\ \tau_1 \end{smallmatrix} \right)$ are known explicitly. An important example is that of *classical, irreversible thermodynamics of stationary, Markov processes in the linear regime*. For such processes one has [66]

$$f_1 \left(\begin{smallmatrix} y_2 \\ \tau_2 \end{smallmatrix} \middle| \begin{smallmatrix} y_1 \\ \tau_1 \end{smallmatrix} \right) = \frac{1}{\sqrt{2\pi}} \frac{s/k_B}{\sqrt{1 - e^{-2\gamma(\tau_2 - \tau_1)}}} \exp \left[-\frac{s}{2k_B} \frac{(y_2 - e^{-\gamma(\tau_2 - \tau_1)}y_1)^2}{1 - e^{-2\gamma(\tau_2 - \tau_1)}} \right]. \quad (4.15)$$

The notation used here is that of [4]. Specifically, k_B is Boltzmann’s constant, the entropy S is a function of the extensive parameter y , and we expand S in a Taylor

series around a stable equilibrium point. Up to quadratic terms we have

$$S = S_0 - \frac{1}{2}sy^2 + \dots, \quad s := -\left.\frac{d^2S}{dy^2}\right|_0 > 0. \quad (4.16)$$

Moreover, the assumption of linearity implies the following proportionality between the thermodynamical force $Y := dS/dy$ and the flux $\dot{y} := dy/d\tau$ it produces [66]:

$$\dot{y} = LY, \quad L > 0. \quad (4.17)$$

The Onsager coefficient L must be positive for the process to be dissipative. Finally $\gamma := sL$. Sometimes one also uses $R := L^{-1}$, so $\gamma = s/R$.

The following path–integral representation for the conditional probabilities (4.15) of these models is noteworthy [66]:

$$f_1 \left(\begin{matrix} y_2 \\ \tau_2 \end{matrix} \middle| \begin{matrix} y_1 \\ \tau_1 \end{matrix} \right) = \int_{y(\tau_1)=y_1}^{y(\tau_2)=y_2} Dy(\tau) \exp \left\{ -\frac{1}{2k_B} \int_{\tau_1}^{\tau_2} d\tau \mathcal{L} [\dot{y}(\tau), y(\tau)] \right\}. \quad (4.18)$$

The above exponential contains the *thermodynamical Lagrangian* \mathcal{L} , defined as

$$\mathcal{L} [\dot{y}(\tau), y(\tau)] := \frac{R}{2} [\dot{y}^2(\tau) + \gamma^2 y^2(\tau)], \quad \dot{y} := \frac{dy}{d\tau}. \quad (4.19)$$

The path integral (4.18) is the thermodynamical analogue of (4.10). The corresponding thermodynamical momentum p_y equals $Rdy/d\tau$, where R plays the role of a mass, and the *thermodynamical Hamiltonian* \mathcal{H} corresponding to (4.19) reads

$$\mathcal{H} = \frac{1}{2R}p_y^2 - \frac{R\gamma^2}{2}y^2. \quad (4.20)$$

It must be borne in mind, however, that the dimensions of \mathcal{L} and \mathcal{H} are entropy per unit time. With this caveat, we will continue to call \mathcal{H} a Hamiltonian.

4.2.4 Mapping thermodynamics into quantum mechanics

For the processes considered in (4.15) we claim that one can define operators on $L^1(\mathbb{R})$ and on $L^\infty(\mathbb{R})$

$$\mathcal{U}(\tau) := \exp \left(-\frac{1}{2k_B} \tau \mathcal{H} \right) \quad (4.21)$$

with \mathcal{H} suitably chosen, such that their matrix elements coincide with those given in (4.14). Hence the $\mathcal{U}(\tau)$ will provide a representation of the algebra (4.13). In what follows we construct $\mathcal{U}(\tau)$ explicitly, but one can already expect the argument \mathcal{H} of the exponential (4.21) to be some *operator* version of the thermodynamical Hamiltonian *function* given in (4.20). For this reason we have not distinguished notationally between the two. This operator \mathcal{H} will also turn out to be (proportional to) the unknown operator A mentioned after eq. (4.14). From (4.21) it follows that the thermodynamical analogue of the quantum–mechanical equation (4.8) is

$$-2k_B \frac{d\mathcal{U}(\tau)}{d\tau} = \mathcal{H}\mathcal{U}(\tau), \quad \mathcal{H} = -2k_B \left. \frac{d\mathcal{U}(\tau)}{d\tau} \right|_{\tau=0}. \quad (4.22)$$

We can resort to our previous work [4] in order to identify the operator \mathcal{H} in its action on $L^1(\mathbb{R})$ and on $L^\infty(\mathbb{R})$. In [4] we have established a map between quantum mechanics in the semiclassical regime, on the one hand, and the theory of classical, irreversible thermodynamics of stationary, Markov processes in the linear regime, on the other hand. In the mechanical picture, the relevant Lagrangian and Hamiltonian functions are

$$L = \frac{m}{2} \left(\frac{dx}{dt} \right)^2 - \frac{m\omega^2}{2} x^2, \quad H = \frac{1}{2m} p_x^2 + \frac{m\omega^2}{2} x^2. \quad (4.23)$$

Comparing them with their thermodynamical partners (4.19) and (4.20), we see that the mechanical and the thermodynamical functions can be transformed into each other if we apply the replacements⁴

$$\omega \leftrightarrow \gamma, \quad \frac{m\omega}{\hbar} \leftrightarrow \frac{s}{2k_B}, \quad x \leftrightarrow y, \quad (4.24)$$

as well as the Wick rotation

$$\tau = it. \quad (4.25)$$

Furthermore, Boltzmann's constant k_B is the thermodynamical partner of Planck's constant \hbar multiplied by 2 [82]:

$$\hbar \leftrightarrow 2k_B. \quad (4.26)$$

As a consistency check one can apply all the above replacements to (4.7) in order to arrive at

$$U(t) = \exp\left(-\frac{i}{\hbar}tH\right) \leftrightarrow \exp\left(-\frac{1}{2k_B}\tau\mathcal{H}\right) = \mathcal{U}(\tau). \quad (4.27)$$

However, we still have to identify the operator \mathcal{H} in its action on thermodynamical states. This will be done in section 4.3.1.

4.2.5 Incoming states vs. outgoing states

In principle, thermodynamical states are normalised probability densities, hence elements of $L^1(\mathbb{R})$. However, as we will see shortly, this viewpoint must be extended somewhat. For this purpose let us call the elements of $L^1(\mathbb{R})$ *incoming states*. Incoming linear operators \mathcal{O}_{in} are defined

$$\mathcal{O}_{\text{in}} : L^1(\mathbb{R}) \longrightarrow L^1(\mathbb{R}), \quad (4.28)$$

so as to map incoming states $|\phi\rangle \in L^1(\mathbb{R})$ into incoming states $\mathcal{O}_{\text{in}}|\phi\rangle \in L^1(\mathbb{R})$. Incoming states are postulated to evolve in time according to

$$-2k_B \frac{d|\phi\rangle}{d\tau} = \mathcal{H}_{\text{in}}|\phi\rangle, \quad (4.29)$$

⁴While the first two replacements in Eq. (4.24) are dimensionally correct without any further assumptions, the third identification also requires that x and y have the same dimensions. Since this need not always be the case, a dimensional conversion factor must be understood as implicitly contained in the replacement $x \leftrightarrow y$, whenever needed.

where \mathcal{H}_{in} is an incoming linear operator, to be identified presently.

The space of outgoing states is the topological dual of $L^1(\mathbb{R})$, hence $L^\infty(\mathbb{R})$. Outgoing linear operators \mathcal{O}_{out} are similarly defined

$$\mathcal{O}_{\text{out}} : L^\infty(\mathbb{R}) \longrightarrow L^\infty(\mathbb{R}), \quad (4.30)$$

in order to map outgoing states $(\psi| \in L^\infty(\mathbb{R})$ into outgoing states $(\psi|\mathcal{O}_{\text{out}} \in L^\infty(\mathbb{R})$. The operator $\mathcal{O}_{\text{in}}^T$ that is transpose to an incoming operator \mathcal{O}_{in} is defined on the topological dual space:

$$\mathcal{O}_{\text{in}}^T : L^\infty(\mathbb{R}) \longrightarrow L^\infty(\mathbb{R}). \quad (4.31)$$

In this way $\mathcal{O}_{\text{in}}^T$ is actually an outgoing operator \mathcal{O}_{out} ⁵. By definition the transpose satisfies

$$(\psi|\mathcal{O}_{\text{in}}^T|\phi) = (\psi|\mathcal{O}_{\text{in}}|\phi), \quad \forall (\psi| \in L^\infty(\mathbb{R}), \forall |\phi) \in L^1(\mathbb{R}). \quad (4.32)$$

What equation should govern the time evolution of outgoing states? Clearly it can only be

$$-2k_B \frac{d(\psi|}{d\tau} = (\psi|\mathcal{H}_{\text{in}}^T = (\psi|\mathcal{H}_{\text{out}}, \quad (4.33)$$

therefore

$$-2k_B \frac{d}{d\tau}(\psi|\phi) = (\psi|\mathcal{H}_{\text{in}}^T|\phi) + (\psi|\mathcal{H}_{\text{in}}|\phi). \quad (4.34)$$

The right-hand side of the above is generally nonzero: it expresses the irreversibility property of time evolution in thermodynamics. This is a far cry from the time-symmetric case of standard quantum mechanics, where $i\hbar d(\langle\psi|\phi\rangle)/dt = 0$.

One further point deserves attention. In standard quantum mechanics on $L^2(\mathbb{R})$, the matrix element $\langle\psi|\mathcal{O}|\phi\rangle = \int dx \psi^*(x)\mathcal{O}\phi(x)$ naturally carries the dimensions of the operator \mathcal{O} ; here both $\psi^*(x)$ and $\phi(x)$ have the dimension $[x]^{-1/2}$ of a probability amplitude on \mathbb{R} . In the thermodynamical dual to quantum theory, the incoming state $|\phi\rangle \in L^1(\mathbb{R})$ carries the dimension $[y]^{-1}$ because it is a probability *density*, while the outgoing state $(\psi| \in L^\infty(\mathbb{R})$ is *dimensionless* because it is *not* meant to be integrated on its own. It is only upon taking the pairing (4.5) that $(\psi|$ will be integrated against $\mathcal{O}|\phi\rangle$. So the dimensions of $(\psi|\mathcal{O}|\phi)$ are again correct, although the dimensional balance between incoming and outgoing states that existed in $L^2(\mathbb{R})$ has disappeared.

Altogether, dispensing with the scalar product in quantum theory is the same as dispensing with time reversal symmetry. Moreover, dispensing with the scalar product has the consequence that, as thermodynamical states, one must regard not just the elements of $L^1(\mathbb{R})$ but also those of its topological dual $L^\infty(\mathbb{R})$.

⁵Since the topological bidual $(L^1(\mathbb{R}))^{**}$ contains more than just $L^1(\mathbb{R})$, we stop short of stating that “The transpose $\mathcal{O}_{\text{out}}^T$ to an outgoing operator \mathcal{O}_{out} is an incoming operator \mathcal{O}_{in} ”. The previous statement, trivially true in finitely many dimensions and still true on $L^2(\mathbb{R})$, no longer holds in our context, with the consequence that twice transposing does not give back the original operator. We will see in section 4.3.2 that this fact has far-reaching implications.

4.3 The thermodynamical oscillator

For mechanics we use the *dimensionless* coordinate $x \in \mathbb{R}$. Then the quantum harmonic oscillator equation on $L^2(\mathbb{R})$ reads

$$\left(-\frac{d^2}{dx^2} + x^2\right)w(x) = \varepsilon w(x), \quad \varepsilon \in \mathbb{R}, \quad (4.35)$$

where ε is a dimensionless energy eigenvalue.

4.3.1 The oscillator on the Banach spaces $L^1(\mathbb{R})$ and $L^\infty(\mathbb{R})$

For thermodynamics we use the *dimensionless* coordinate $y \in \mathbb{R}$. Then the dimensionless thermodynamical momentum is represented as $-i\mathrm{d}/\mathrm{d}y$, and the equation for the thermodynamical oscillator reads

$$-\left(\frac{d^2}{dy^2} + y^2\right)w(y) = \sigma w(y) \quad \sigma \in \mathbb{R}. \quad (4.36)$$

Above, σ is a dimensionless eigenvalue (entropy per unit time), which we require to be real for physical reasons. With respect to (4.35), the only change in (4.36) is the sign of the potential term (see (4.19) and (4.20)). Eq. (4.36) identifies the operator \mathcal{H} explicitly in its action on $L^1(\mathbb{R})$ and $L^\infty(\mathbb{R})$, a question posed in section 4.2.4. Specifically, for the action of the Hamiltonian on the initial states we have

$$\mathcal{H}_{\mathrm{in}} = -\frac{d^2}{dy^2} - y^2 : L^1(\mathbb{R}) \longrightarrow L^1(\mathbb{R}). \quad (4.37)$$

The operator $\mathcal{H}_{\mathrm{out}}$ is formally the same as $\mathcal{H}_{\mathrm{in}}$, but it acts on the dual space:

$$\mathcal{H}_{\mathrm{out}} = -\frac{d^2}{dy^2} - y^2 : L^\infty(\mathbb{R}) \longrightarrow L^\infty(\mathbb{R}). \quad (4.38)$$

In order to solve (4.36) we first look for a factorisation of $w(y)$ in the form

$$w(y) = h(y) \exp(\alpha y^2), \quad \alpha \in \mathbb{C}, \quad (4.39)$$

where α is some constant to be picked appropriately. With (4.39) in (4.36) one finds

$$\frac{d^2}{dy^2}h(y) + 4\alpha y \frac{d}{dy}h(y) + [(2\alpha + \sigma) + (4\alpha^2 + 1)y^2]h(y) = 0. \quad (4.40)$$

The choice $\alpha = i/2$ simplifies (4.40) considerably:

$$\frac{d^2}{dy^2}h(y) + 2iy \frac{d}{dy}h(y) + (i + \sigma)h(y) = 0. \quad (4.41)$$

Finally the change of variables $z = e^{i\frac{3\pi}{4}} y$ reduces (4.41) to

$$\frac{d^2}{dz^2} \tilde{h}(z) - 2z \frac{d}{dz} \tilde{h}(z) - (1 - i\sigma) \tilde{h}(z) = 0, \quad (4.42)$$

where we have defined $\tilde{h}(z) := h\left(e^{-i\frac{3\pi}{4}} z\right) = h(y)$. Now (4.42) is a particular instance of the Hermite differential equation on the complex plane,

$$H''(z) - 2zH'(z) + 2\nu H(z) = 0, \quad \nu \in \mathbb{C}. \quad (4.43)$$

In our case we have $2\nu = -1 + i\sigma$ with $\sigma \in \mathbb{R}$, so $\nu \notin \mathbb{N}$. When $\nu \notin \mathbb{N}$ two linearly independent solutions to the Hermite equation are given by the Hermite functions $H_\nu(z)$ and $H_\nu(-z)$, where [60]

$$H_\nu(z) = \frac{1}{2\Gamma(-\nu)} \sum_{n=0}^{\infty} \frac{(-1)^n \Gamma\left(\frac{n-\nu}{2}\right)}{n!} (2z)^n. \quad (4.44)$$

The above power series defines an entire function of $z \in \mathbb{C}$ for any value of $\nu \in \mathbb{C}$. Its asymptotic behaviour is [60]:

$$H_\nu(z) \sim (2z)^\nu - \frac{\sqrt{\pi} e^{i\pi\nu}}{\Gamma(-\nu)} z^{-\nu-1} e^{z^2}, \quad |z| \rightarrow \infty, \quad \pi/4 < \arg(z) < 5\pi/4. \quad (4.45)$$

In (4.45) we have dropped subdominant terms, keeping only the leading contributions; the angular sector $\pi/4 < \arg(z) < 5\pi/4$ is imposed on us by the change of variables $z = e^{i\frac{3\pi}{4}} y$ made above for $y \in \mathbb{R}$.

Altogether, two linearly independent solutions to (4.36) corresponding to the eigenvalue $\sigma \in \mathbb{R}$ are given by $w_\sigma^\pm(y)$, where

$$w_\sigma^\pm(y) := H_{-\frac{1}{2} + \frac{i\sigma}{2}}\left(\pm e^{i\frac{3\pi}{4}} y\right) e^{iy^2/2}. \quad (4.46)$$

By (4.45), their asymptotic behaviour for $|y| \rightarrow \infty$ is

$$w_\sigma^\pm(y) \sim \left(\pm 2e^{i\frac{3\pi}{4}} y\right)^{-\frac{1}{2} + \frac{i\sigma}{2}} e^{iy^2/2} - \frac{\sqrt{\pi} e^{-\pi(\sigma+i)/2}}{\Gamma\left(\frac{1-i\sigma}{2}\right)} \left(\pm e^{i\frac{3\pi}{4}} y\right)^{-\frac{1}{2} - \frac{i\sigma}{2}} e^{-iy^2/2}. \quad (4.47)$$

We are looking for eigenfunctions within $L^1(\mathbb{R})$ and/or $L^\infty(\mathbb{R})$. Eqn. (4.47) proves that $w_\sigma^\pm(y) \in L^\infty(\mathbb{R})$ but $w_\sigma^\pm(y) \notin L^1(\mathbb{R})$.

4.3.2 The point spectrum of real eigenvalues

Summarising, the operator $-d^2/dy^2 - y^2$ on $L^\infty(\mathbb{R})$ has a point spectrum containing the whole real line \mathbb{R} .⁶ This subset (the real line \mathbb{R}) of the point spectrum is twice degenerate, the (unnormalised) eigenfunctions corresponding to $\sigma \in \mathbb{R}$ being given in Eq.

⁶Here we are restricting our attention to the *point spectrum*; for our purposes we need not compute the full spectrum. Although the point spectrum of our operator on $L^\infty(\mathbb{R})$ also contains nonreal eigenvalues (see Eq. (4.48)), for physical reasons explained in the text we are only interested in real eigenvalues.

(4.46). The same operator acting on $L^1(\mathbb{R})$ has a void point spectrum. This latter conclusion is not as tragic as it might seem at first sight—on the contrary, everything fits together once one realises that evolution in thermodynamical time τ is irreversible, and that the space $L^1(\mathbb{R})$, which admits a Schauder basis, has a topological dual $L^\infty(\mathbb{R})$ admitting no Schauder basis. Let us analyse these facts from a physical and from a mathematical viewpoint.

Physically, an empty point spectrum on $L^1(\mathbb{R})$ just means that *there can be no incoming eigenstates*. Moreover, no incoming state can ever evolve into an incoming *eigenstate* under thermodynamical evolution. This is an expression of irreversibility. However, as a result of evolution in τ , one can perfectly well obtain *outgoing* eigenstates. The latter remain outgoing *eigenstates* under thermodynamical evolution.

Mathematically, in standard quantum mechanics on $L^2(\mathbb{R})$ one is used to taking the transpose of a matrix by exchanging rows with columns. Implicitly understood here is the existence of Schauder bases in the space of $L^2(\mathbb{R})$ and in its topological dual (again $L^2(\mathbb{R})$). Once one diagonalises an operator, how can it be that its transpose is not diagonal as well? While this cannot happen in $L^2(\mathbb{R})$, *this can perfectly well be the case when dealing with the spaces $L^1(\mathbb{R})$ and $L^\infty(\mathbb{R})$, because $L^1(\mathbb{R})$ admits a Schauder basis while $L^\infty(\mathbb{R})$ does not*. In turn, this is a consequence of the fact that we are renouncing probability density *amplitudes* (elements of $L^2(\mathbb{R})$) in favour of probability *densities* (elements of $L^1(\mathbb{R})$), as befits a thermodynamical description of quantum theory.

One would like to identify the thermodynamical analogue of the quantum mechanical vacuum state; one expects to somehow map the quantum–mechanical state of least energy, or vacuum, into the thermodynamical state of maximal entropy. Let us recall that the (unnormalised) quantum–mechanical vacuum wavefunction is $\exp(-x^2/2)$. The Wick rotation (4.25) introduces the imaginary unit, giving us the term $\exp(iy^2/2)$ in (4.46). Now $\nu = -1/2 + i\sigma/2 = 0$ only when $\sigma = -i$, a possibility we have excluded per decree. Let us temporarily sidestep this decree and observe that

$$-\left(\frac{d^2}{dy^2} + y^2\right)e^{\pm iy^2/2} = \mp i e^{\pm iy^2/2} \quad (4.48)$$

is very reminiscent of the equation governing the quantum–mechanical vacuum. The thermodynamical density corresponding to the state $\exp(\pm iy^2/2)$ equals the constant unit function on \mathbb{R} , which is nonnormalisable under $\|\cdot\|_1$ in $L^1(\mathbb{R})$ but carries finite norm under $\|\cdot\|_\infty$ in $L^\infty(\mathbb{R})$. As a perfectly uniform probability distribution, $\exp(\pm iy^2/2)$ is *the thermodynamical state that maximises the entropy*. All the eigenstates in (4.46) are thermodynamical excitations thereof, hence they carry less entropy. Of course, we cannot allow the eigenvalues $\sigma = \pm i$ within our point spectrum, but the above discussion is illustrative because, by Eq. (4.47), all our thermodynamical eigenstates (4.46) tend asymptotically to the states $y^{-1/2} \exp[\pm \frac{i}{2}(\sigma \ln(y) + y^2)]$ (or linear combinations thereof). In other words, all our thermodynamical eigenstates can be interpreted as *fluctuations around a state of maximal entropy*.

4.3.3 Irreversibility vs. nonunitarity

A key consequence of irreversibility is nonunitarity. Contrary to the operators $U(t)$ of (4.7), which are unitary on $L^2(\mathbb{R})$, the operators $\mathcal{U}(\tau)$ of (4.21) are *nonunitary* on $L^\infty(\mathbb{R})$.

Nonunitarity is readily proved. Let $w_\sigma \in L^\infty(\mathbb{R})$ be such that $\mathcal{H}_{\text{out}} w_\sigma = \sigma w_\sigma$. Since $\sigma \in \mathbb{R}$ we have, by (4.21),

$$\mathcal{U}(\tau)w_\sigma = \exp\left(-\frac{\tau\sigma}{2k_B}\right)w_\sigma, \quad \tau\sigma \in \mathbb{R}, \quad (4.49)$$

hence

$$\|\mathcal{U}(\tau)w_\sigma\|_\infty = \exp\left(-\frac{\tau\sigma}{2k_B}\right)\|w_\sigma\|_\infty, \quad \tau\sigma \in \mathbb{R}, \quad (4.50)$$

which proves our assertion. To summarise: combining (4.21), (4.37) and (4.38) we find, after reinstating dimensional factors, that the operators

$$\mathcal{U}(\tau) = \exp\left[\frac{\tau}{2k_B}\left(\frac{1}{2R}\frac{d^2}{dy^2} + \frac{R\gamma^2}{2}y^2\right)\right], \quad \tau \geq 0, \quad (4.51)$$

provide a *nonunitary*, infinite-dimensional representation of the Chapman–Kolmogorov semigroup (4.13) on $L^\infty(\mathbb{R})$. The space $L^1(\mathbb{R})$ also carries an infinite-dimensional representation of (4.13) on which the operators (4.51) act.

It is interesting to observe that the eigenfunctions in (4.48), which we have discarded for reasons already explained, circumvent the above proof because their eigenvalues are purely imaginary. Each one of them actually provides a 1-dimensional, *unitary* representation of (4.13) on $L^\infty(\mathbb{R})$.

4.4 Conclusions to chapter 4

Classical thermodynamics is the paradigm of emergent theories. It renounces the detailed knowledge of a large number of microscopic degrees of freedom, in favour of a small number of macroscopic averages that retain only some coarse-grained features of the system under consideration. It has been claimed in the literature that quantum mechanics must be an emergent theory [5, 13, 49]. As one further piece of evidence in support of this latter statement, in this paper we have developed a thermodynamical formalism for quantum mechanics.

In the usual formulation of quantum theory, one is concerned with the matrix elements $\langle\psi|\mathcal{O}|\phi\rangle$ of some operator \mathcal{O} , where the incoming state $|\phi\rangle$ belongs to $L^2(\mathbb{R})$ and the outgoing state $\langle\psi|$ belongs to the topological dual space, again $L^2(\mathbb{R})$.

In the thermodynamical theory that is dual to quantum mechanics one is again concerned with matrix elements of the type $(\psi|\mathcal{O}|\phi)$. However, now the incoming state

is not square integrable but just integrable, $|\phi\rangle \in L^1(\mathbb{R})$, while the outgoing state $\langle\psi| \in L^\infty(\mathbb{R})$ belongs to a totally different space. Neither $L^1(\mathbb{R})$ nor its topological dual $L^\infty(\mathbb{R})$ qualify as a Hilbert space, because their respective norms do not derive from a scalar product; they are just Banach spaces. The absence of a scalar product is the hallmark of irreversibility. Indeed the thermodynamics that is dual to quantum mechanics is that of irreversible processes (considered here in the linear regime).

One is often interested in the case when the operator \mathcal{O} is the time evolution operator \mathcal{U} connecting the incoming and the outgoing states. Not being allowed to exchange the incoming and the outgoing *states* in the transition probability $\langle\psi|\mathcal{U}|\phi\rangle$, because they belong to different spaces, emphasis falls on the *process* \mathcal{U} connecting these two. Irreversibility manifests itself through the nonunitarity of the representation constructed here for the Chapman–Kolmogorov equation. The latter is the functional equation satisfied by \mathcal{U} .

Incoming states $|\phi\rangle \in L^1(\mathbb{R})$ are probability densities, as opposed to the probability density *amplitudes* $|\phi\rangle \in L^2(\mathbb{R})$ of standard quantum theory. Outgoing states $\langle\psi| \in L^\infty(\mathbb{R})$ have a different physical interpretation. The norm $\|\cdot\|_\infty$ can be regarded as a probability density that is *not* meant to be integrated. Indeed a general function $\psi \in L^\infty(\mathbb{R})$ need not be normalisable under the norms $\|\cdot\|_1$ and $\|\cdot\|_2$ on $L^1(\mathbb{R})$ and $L^2(\mathbb{R})$ respectively. There is nothing unusual about this—scattering states in standard quantum theory also give rise to nonnormalisable probability densities.

As an example, in section 4.3.1 we have worked out the point spectrum for the thermodynamical harmonic oscillator. This implies solving the Schroedinger equation for the *repulsive* potential $V(y) = -y^2$, the wrong sign being due to the Wick rotation connecting irreversible thermodynamics to mechanics. Not surprisingly, the point spectrum is empty when diagonalising the Hamiltonian on the space $L^1(\mathbb{R})$, while exhibiting rich features on the space $L^\infty(\mathbb{R})$. In particular, all our eigenstates turn out to be nonnormalisable under the norms $\|\cdot\|_1$ and $\|\cdot\|_2$ on $L^1(\mathbb{R})$ and $L^2(\mathbb{R})$ respectively, hence they all are analogous to scattering states in standard quantum theory. However all our eigenstates are normalisable under the norm $\|\cdot\|_\infty$ of $L^\infty(\mathbb{R})$.

An apparently striking feature is the reluctance of incoming states to build *eigenstates* of the Hamiltonian, as seen in section 4.3.2. This apparent difficulty disappears once one realises that *outgoing* states make perfectly good eigenstates. Furthermore, the existence of outgoing states that cannot be reached by the time evolution of any incoming state whatsoever is another sign of irreversibility. We cannot renounce irreversibility because we have programatically dispensed with time reversal symmetry. Hence incoming eigenstates must go.

Chapter 5

Overall summary

A very brief summary of the points analysed in this PhD thesis could be as follows:

i) In chapter 2, the emergent nature of quantum mechanics is shown to follow from a precise correspondence with the classical theory of irreversible thermodynamics. Specifically, the linear (or Gaussian) regime of the latter can be put in a 1-to-1 map with the semiclassical approximation to quantum mechanics. The very possibility of reinterpreting quantum mechanics as a thermodynamics proves that the former is an emergent phenomenon. That is, quantum mechanics is a coarse-grained description of some underlying degrees of freedom.

ii) In chapter 3 we start recalling that it has been argued that gravity acts dissipatively on quantum-mechanical systems, inducing thermal fluctuations that become indistinguishable from quantum fluctuations. This has led some authors to demand that some form of time irreversibility be incorporated into the formalism of quantum mechanics. As a tool towards this goal we propose a thermodynamical approach to quantum mechanics, based on Onsager's classical theory of irreversible processes and on Prigogine's nonunitary transformation theory. An entropy operator replaces the Hamiltonian as the generator of evolution. The canonically conjugate variable corresponding to the entropy is a dimensionless evolution parameter. Contrary to the Hamiltonian, the entropy operator is not a conserved Noether charge. Our construction succeeds in implementing gravitationally-induced irreversibility in the quantum theory.

iii) In chapter 4 we have elaborated on the existing notion that quantum mechanics is an emergent phenomenon, by presenting a thermodynamical theory that is dual to quantum mechanics. This dual theory is that of classical irreversible thermodynamics. The linear regime of irreversibility considered here corresponds to the semiclassical approximation in quantum mechanics. An important issue we address is how the irreversibility of time evolution in thermodynamics is mapped onto the quantum-mechanical side of the correspondence.

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