

# BETWEEN CLASSICAL AND QUANTUM

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‘But the worst thing is that I am quite unable to clarify the transition [of matrix mechanics] to the classical theory.’ [Heisenberg to Pauli, October 23th, 1925]<sup>1</sup>

‘Hendrik Lorentz considered the establishment of the correct relation between the classical and the quantum theory as the most fundamental problem of future research. This problem bothered him as much as it did Planck.’ [Mehra and Rechenberg, 2000, 721]

‘Thus quantum mechanics occupies a very unusual place among physical theories: it contains classical mechanics as a limiting case, yet at the same time it requires this limiting case for its own formulation.’ [Landau and Lifshitz, 1977, 3]

## 1 INTRODUCTION

Most modern physicists and philosophers would agree that a decent interpretation of quantum mechanics should fulfil at least two criteria. Firstly, it has to elucidate the physical meaning of its mathematical formalism and thereby secure the empirical content of the theory. This point (which we address only in a derivative way) was clearly recognized by all the founders of quantum theory.<sup>2</sup> Secondly (and this *is* the subject of this paper), it has to explain at least the *appearance* of the classical world.<sup>3</sup> As shown by our second quotation above, Planck saw the difficulty this poses, and as a first contribution he noted that the high-temperature

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<sup>1</sup>‘Aber das Schlimmste ist, daß ich über den Übergang in die klassische Theorie nie Klarheit bekommen kann.’ See [Pauli, 1979, 251].

<sup>2</sup>The history of quantum theory has been described in a large number of books. The most detailed presentation is in [Mehra and Rechenberg, 1982–2001], but this multi-volume series has by no means superseded smaller works such as [Jammer, 1966; van der Waerden, 1967; Hendry, 1984; Darrigol, 1992], and [Beller, 1999]. Much information may also be found in biographies such as [Heisenberg, 1969; Pais, 1982; Moore, 1989; Pais, 1991; Cassidy, 1992; Heilbron, 2000; Enz, 2002], etc. See also [Pauli, 1979]. A new project on the history of matrix mechanics led by Jürgen Renn is on its way.

<sup>3</sup>That these points are quite distinct is shown by the Copenhagen Interpretation, which exclusively addresses the first at utter neglect of the second. Nonetheless, in most other approaches to quantum mechanics there is substantial overlap between the various mechanisms that are proposed to fulfil the two criteria in question.

limit of his formula for black-body radiation converged to the classical expression. Although Bohr believed that *quantum mechanics should be interpreted through classical physics*, among the founders of the theory he seems to have been unique in his lack of appreciation of the problem of *deriving classical physics from quantum theory*. Nonetheless, through his correspondence principle (which he proposed in order to address the *first* problem above rather than the second) Bohr made one of the most profound contributions to the issue. Heisenberg initially recognized the problem, but quite erroneously came to believe he had solved it in his renowned paper on the uncertainty relations.<sup>4</sup> Einstein famously did not believe in the fundamental nature of quantum theory, whereas Schrödinger was well aware of the problem from the beginning, later highlighted the issue with his legendary cat, and at various stages in his career made important technical contributions towards its resolution. Ehrenfest stated the well-known theorem named after him. Von Neumann saw the difficulty, too, and addressed it by means of his well-known analysis of the measurement procedure in quantum mechanics.

The problem is actually even more acute than the founders of quantum theory foresaw. The experimental realization of Schrödinger's cat is nearer than most physicists would feel comfortable with [Leggett, 2002; Brezger *et al.*, 2002; Chiorescu *et al.*, 2003; Marshall *et al.*, 2003; Devoret *et al.*, 2004]. Moreover, awkward superpositions are by no means confined to physics laboratories: due to its chaotic motion, Saturn's moon Hyperion (which is about the size of New York) has been estimated to spread out all over its orbit within 20 years if treated as an isolated quantum-mechanical wave packet [Zurek and Paz, 1995]. Furthermore, decoherence theorists have made the point that "measurement" is not only a procedure carried out by experimental physicists in their labs, but takes place in Nature all the time without any human intervention. On the conceptual side, parties as diverse as Bohm and Bell and their followers on the one hand and the quantum cosmologists on the other have argued that a "Heisenberg cut" between object and observer cannot possibly lie at the basis of a fundamental theory of physics.<sup>5</sup> These and other remarkable insights of the past few decades have drawn wide attention to the importance of the problem of interpreting quantum mechanics, and in particular of explaining classical physics from it.

We will discuss these ideas in more detail below, and indeed our discussion of the relationship between classical and quantum mechanics will be partly historical. However, other than that it will be technical and mathematically rigorous. For the problem at hand is so delicate that in this area sloppy mathematics is almost guaranteed to lead to unreliable physics and conceptual confusion (notwithstand-

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<sup>4</sup>One can see that the transition from micro- to macro-mechanics is now very easy to understand: classical mechanics is altogether part of quantum mechanics.' (Heisenberg to Bohr, 19 March 1927, just before the submission on 23 March of Heisenberg [1927]. See *Bohr's Scientific Correspondence in the Archives for the History of Quantum Physics*).

<sup>5</sup>Not to speak of the problem, also raised by quantum cosmologists, of deriving classical space-time from some theory of quantum gravity. This is certainly part of the general program of deriving classical physics from quantum theory, but unfortunately it cannot be discussed in this paper.

ing the undeniable success of poor man's math elsewhere in theoretical physics). Except for von Neumann, this was not the attitude of the pioneers of quantum mechanics; but while it has to be acknowledged that many of their ideas are still central to the current discussion, these ideas *per se* have *not* solved the problem. Thus we assume the reader to be familiar with the Hilbert space formalism of quantum mechanics,<sup>6</sup> and for some parts of this paper (notably Section 6 and parts of Section 4) also with the basic theory of  $C^*$ -algebras and its applications to quantum theory.<sup>7</sup> In addition, some previous encounter with the conceptual problems of quantum theory would be helpful.<sup>8</sup>

Which ideas *have* solved the problem of explaining the appearance of the classical world from quantum theory? In our opinion, none have, although since the founding days of quantum mechanics a number of new ideas have been proposed that almost certainly will play a role in the eventual resolution, should it ever be found. These ideas surely include:

- The limit  $\hbar \rightarrow 0$  of small Planck's constant (coming of age with the mathematical field of microlocal analysis);
- The limit  $N \rightarrow \infty$  of a large system with  $N$  degrees of freedom (studied in a serious way only after the emergence of  $C^*$ -algebraic methods);
- Decoherence and consistent histories.

Mathematically, the second limit may be seen as a special case of the first, though the underlying physical situation is of course quite different. In any case, after a detailed analysis our conclusion will be that none of these ideas in isolation is capable of explaining the classical world, but that there is some hope that by combining all three of them, one might do so in the future.

Because of the fact that the subject matter of this review is unfinished business, to date one may adopt a number of internally consistent but mutually incompatible philosophical stances on the relationship between classical and quantum theory. Two extreme ones, which are always useful to keep in mind whether one holds one of them or not, are:

1. Quantum theory is fundamental and universally valid, and the classical world has only "relative" or "perspectival" existence.
2. Quantum theory is an approximate and derived theory, possibly false, and the classical world exists absolutely.

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<sup>6</sup>Apart from seasoned classics such as [Mackey, 1963; Jauch, 1968; Prugovecki, 1971; Reed and Simon, 1972], or [Thirring, 1981], the reader might consult more recent books such as [Gustafson and Sigal, 2003] or [Williams, 2003]. See also [Dickson, 2005].

<sup>7</sup>For physics-oriented introductions to  $C^*$ -algebras see [Davies, 1976; Roberts and Roepstorff, 1969; Primas, 1983; Thirring, 1983; Emch, 1984; Strocchi, 1985; Sewell, 1986; Roberts, 1990; Haag, 1992; Landsman, 1998; Araki, 1999], and [Sewell, 2002]. Authoritative mathematical texts include [Kadison and Ringrose, 1983; 1986] and [Takesaki, 2003].

<sup>8</sup>Trustworthy books include, for example, [Scheibe, 1973; Jammer, 1974; van Fraassen, 1991; d'Espagnat, 1995; Peres, 1995; Omnès, 1994; 1999; Bub, 1997], and [Mittelstaedt, 2004].

An example of a position that our modern understanding of the measurement problem<sup>9</sup> has rendered internally inconsistent is:

3. Quantum theory is fundamental and universally valid, and (yet) the classical world exists absolutely.

In some sense stance 1 originates with Heisenberg [1927], but the modern era started with Everett [1957].<sup>10</sup> These days, most decoherence theorists, consistent historians, and modal interpreters seem to support it. Stance 2 has a long and respectable pedigree unequivocally, including among others Einstein, Schrödinger, and Bell. More recent backing has come from Leggett as well as from “spontaneous collapse” theorists such as Pearle, Ghirardi, Rimini, Weber, and others. As we shall see in Section 3, Bohr’s position eludes classification according to these terms; our three stances being of an ontological nature, he probably would have found each of them unattractive.

Of course, one has to specify what the terminology involved means. By quantum theory we mean standard quantum mechanics including the eigenvector-eigenvalue link.<sup>11</sup> Modal interpretations of quantum mechanics [Dieks, 1989a; 1989b; van Fraassen, 1991; Bub, 1999; Vermaas, 2000; Bene & Dieks, 2002; Dickson, 2005] deny this link, and lead to positions close to or identical to stance 1. The projection postulate is neither endorsed nor denied when we generically speak of quantum theory.

It is a bit harder to say what “the classical world” means. In the present discussion we evidently can *not* define the classical world as the world that exists independently of observation – as Bohr did, see Subsection 3.1 – but neither can it be taken to mean the part of the world that is described by the laws of classical physics full stop; for if stance 1 is correct, then these laws are only approximately valid, if at all. Thus we simply put it like this:

*The classical world is what observation shows us to behave – with appropriate accuracy – according to the laws of classical physics.*

There should be little room for doubt as to what ‘with appropriate accuracy’ means: the existence of the colour grey does not imply the nonexistence of black and white!

We *can* define the *absolute existence* of the classical world à la Bohr as its existence independently of observers or measuring devices. Compare with Moore’s [1939] proof of the existence of the external world:

<sup>9</sup>See the books cited in footnote 8, especially [Mittelstaedt, 2004].

<sup>10</sup>Note, though, that stance 1 by no means implies the so-called Many-Worlds Interpretation, which also in our opinion is ‘simply a meaningless collage of words’ [Leggett, 2002].

<sup>11</sup>Let  $A$  be a selfadjoint operator on a Hilbert space  $\mathcal{H}$ , with associated projection-valued measure  $P(\Delta)$ ,  $\Delta \subset \mathbb{R}$ , so that  $A = \int dP(\lambda) \lambda$  (see also footnote 99 below). The eigenvector-eigenvalue link states that a state  $\Psi$  of the system lies in  $P(\Delta)\mathcal{H}$  if and only if  $A$  takes some value in  $\Delta$  for sure. In particular, if  $\Psi$  is an eigenvector of  $A$  with eigenvalue  $\lambda$  (so that  $P(\{\lambda\}) \neq 0$  and  $\Psi \in P(\{\lambda\})\mathcal{H}$ ), then  $A$  takes the value  $\lambda$  in the state  $\Psi$  with probability one. In general, the probability  $p_\Psi(\Delta)$  that in a state  $\Psi$  the observable  $a$  takes some value in  $\Delta$  (“upon measurement”) is given by the Born–von Neumann rule  $p_\Psi(\Delta) = (\Psi, P(\Delta)\Psi)$ .

How? By holding up my two hands, and saying, as I make a certain gesture with the right hand, ‘Here is one hand’, and adding, as I make a certain gesture with the left, ‘and here is another’.

Those holding position 1, then, maintain that *the classical world exists only as an appearance relative to a certain specification*, where the specification in question could be an observer (Heisenberg), a certain class of observers and states (as in decoherence theory), or some coarse-graining of the Universe defined by a particular consistent set of histories, etc. If the notion of an observer is construed in a sufficiently abstract and general sense, one might also formulate stance 1 as claiming that the classical world merely exists *from the perspective of the observer* (or the corresponding class of observables).<sup>12</sup> For example, Schrödinger’s cat “paradox” dissolves at once when the appropriate perspective is introduced; cf. Subsection 6.6.

Those holding stance 2, on the other hand, believe that the classical world exists in an absolute sense (as Moore did). Thus stance 2 is akin to common-sense realism, though the distinction between 1 and 2 is largely independent of the issue of scientific realism.<sup>13</sup> For defendants of stance 1 usually still believe in the existence of some observer-independent reality (namely somewhere in the quantum realm), but deny that this reality incorporates the world observed around us. This justifies a pretty vague specification of such an important notion as the classical world: one of the interesting outcomes of the otherwise futile discussions surrounding the Many Worlds Interpretation has been the insight that *if quantum mechanics is fundamental, then the notion of a classical world is intrinsically vague and approximate*. Hence it would be self-defeating to be too precise at this point.<sup>14</sup>

Although stance 1 is considered defensive if not cowardly by adherents of stance 2, it is a highly nontrivial mathematical fact that so far it seems supported by the formalism of quantum mechanics. In his derision of what he called ‘FAPP’ (= For All Practical Purposes) solutions to the measurement problem (and more general attempts to explain the appearance of the classical world from quantum theory), Bell [1987; 2001] and others in his wake mistook a profound epistemological stance for a poor defensive move.<sup>15</sup> It is, in fact, stance 2 that we would recommend to the cowardly: for proving or disproving stance 1 seems the real challenge of the

<sup>12</sup>The terminology “perspectival” was suggested to the author by Richard Healey.

<sup>13</sup>See [Landsman, 1995] for a more elaborate discussion of realism in this context. Words like “objective” or “subjective” are not likely to be helpful in drawing the distinction either: the claim that ‘my children are the loveliest creatures in the world’ is at first glance subjective, but it can trivially be turned into an objective one through the reformulation that ‘Klaas Landsman finds his children the loveliest creatures in the world’. Similarly, the proposition that (perhaps due to decoherence) ‘local observers find that the world is classical’ is perfectly objective, although it describes a subjective experience. See also [Davidson, 2001].

<sup>14</sup>See [Wallace, 2002; 2003]; also cf. [Butterfield, 2002]. This point was not lost on Bohr and Heisenberg either; see [Scheibe, 1973].

<sup>15</sup>The insistence on “precision” in such literature is reminiscent of Planck’s long-held belief in the absolute nature of irreversibility [Darrigol, 1992; Heilbron, 2002]. It should be mentioned that although Planck’s stubbornness by historical accident led him to take the first steps towards quantum theory, he eventually gave it up to side with Boltzmann.

entire debate, and we regard the technical content of this paper as a survey of progress towards actually proving it. Indeed, to sum up our conclusions, we claim that there is good evidence that:

1. Classical physics emerges from quantum theory in the limit  $\hbar \rightarrow 0$  or  $N \rightarrow \infty$  *provided that the system is in certain “classical” states and is monitored with “classical” observables only*;
2. Decoherence and consistent histories will probably explain *why* the system happens to be in such states and has to be observed in such a way.

However, even if one fine day this scheme will be made to work, the explanation of the appearance of the classical world from quantum theory will be predicated on an external solution of the notorious ‘from “and” to “or” problem’: If quantum mechanics predicts various possible outcomes with certain probabilities, why does only *one* of these appear to us?<sup>16</sup>

For a more detailed outline of this paper we refer to the table of contents above. Most philosophical discussion will be found in Section 3 on the Copenhagen interpretation, since whatever its merits, it has undeniably set the stage for the entire discussion on the relationship between classical and quantum.<sup>17</sup> The remainder of the paper will be of an almost purely technical nature. Beyond this point we will try to avoid controversy, but when unavoidable it will be confined to the Epilogues appended to Sections 3-6. The final Epilogue (Section 8) expresses our deepest thoughts on the subject.

## 2 EARLY HISTORY

This section is a recapitulation of the opinions and contributions of the founders of quantum mechanics regarding the relationship between classical and quantum. More detail may be found in the books cited in footnote 2 and in specific literature to be cited; for an impressive (but incomplete) bibliography see also [Gutzwiller, 1998]. The early history of quantum theory is of interest in its own right, concerned as it is with one of the most significant scientific revolutions in history. Although this history is not a main focus of this paper, it is of special significance for our theme. For the usual and mistaken interpretation of Planck’s work (i.e. the idea that he introduced something like a “quantum postulate”, see Subsection 3.2 below) appears to have triggered the belief that quantum theory and Planck’s constant are related to a universal discontinuity in Nature. Indeed, this discontinuity is sometimes even felt to mark the basic difference between classical and quantum physics. This belief is particularly evident in the writings of Bohr, but still resonates even today.

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<sup>16</sup>It has to be acknowledged that we owe the insistence on this question to the defendants of stance 2. See also footnote 10.

<sup>17</sup>We do not discuss the classical limit of quantum mechanics in the philosophical setting of theory reduction and intertheoretic relations; see, e.g., [Scheibe, 1999] and [Batterman, 2002].

## 2.1 Planck and Einstein

The relationship between classical physics and quantum theory is so subtle and confusing that historians and physicists cannot even agree about the precise way the classical gave way to the quantum! As Darrigol [2001] puts it: ‘During the past twenty years, historians [and physicists] have disagreed over the meaning of the quanta which Max Planck introduced in his black-body theory of 1900. The source of this confusion is the publication (...) of Thomas Kuhn’s [1978] iconoclastic thesis that Planck did not mean his energy quanta to express a quantum discontinuity.’

As is well known (cf. [Mehra and Rechenberg, 1982a], etc.), Planck initially derived Wien’s law for blackbody radiation in the context of his (i.e. Planck’s) program of establishing the absolute nature of irreversibility (competing with Boltzmann’s probabilistic approach, which eventually triumphed). When new high-precision measurements in October 1900 turned out to refute Wien’s law, Planck first guessed his expression

$$(1) \quad E_\nu/N_\nu = h\nu/(e^{h\nu/kT} - 1)$$

for the correct law, *en passant* introducing two new constants of nature  $h$  and  $k$ ,<sup>18</sup> and subsequently, on December 14, 1900, presented a theoretical derivation of his law in which he allegedly introduced the idea that the energy of the resonators making up his black body was quantized in units of  $\varepsilon_\nu = h\nu$  (where  $\nu$  is the frequency of a given resonator). This derivation is generally seen as the birth of quantum theory, with the associated date of birth just mentioned.

However, it is clear by now [Kuhn, 1978; Darrigol, 1992; 2001; Carson, 2000; Brush, 2002] that Planck was at best agnostic about the energy of his resonators, and at worst assigned them a continuous energy spectrum. Technically, in the particular derivation of his empirical law that eventually turned out to lead to the desired result (which relied on Boltzmann’s concept of entropy),<sup>19</sup> Planck had to count the number of ways a given amount of energy  $E_\nu$  could be distributed over a given number of resonators  $N_\nu$  at frequency  $\nu$ . This number is, of course, infinite, hence in order to find a finite answer Planck followed Boltzmann in breaking up  $E_\nu$  into a large number  $A_\nu$  of portions of identical size  $\varepsilon_\nu$ , so that  $A_\nu\varepsilon_\nu = E_\nu$ .<sup>20</sup> Now, as we all know, whereas Boltzmann let  $\varepsilon_\nu \rightarrow 0$  at the end of his corresponding calculation for a gas, Planck discovered that his empirical blackbody law emerged if he assumed the relation  $\varepsilon_\nu = h\nu$ .

However, this postulate did *not* imply that Planck quantized the energy of his resonators. In fact, in his definition of a given distribution he counted the number of resonators with energy *between* say  $(k - 1)\varepsilon_\nu$  and  $k\varepsilon_\nu$  (for some  $k \in$

<sup>18</sup>Hence Boltzmann’s constant  $k$  was introduced by Planck, who was the first to write down the formula  $S = k \log W$ .

<sup>19</sup>Despite the fact that Planck only converted to Boltzmann’s approach to irreversibility around 1914.

<sup>20</sup>The number in question is then given by  $(N + A - 1)/(N - 1)!A!$ , dropping the dependence on  $\nu$  in the notation.

N), as Boltzmann did in an analogous way for a gas, rather than the number of resonators with energy  $k\varepsilon_\nu$ , as most physicists came to interpret his procedure. More generally, there is overwhelming textual evidence that Planck himself by no means believed or implied that he had quantized energy; for one thing, in his Nobel Prize Lecture in 1920 he attributed the correct interpretation of the energy-quanta  $\varepsilon_\nu$  to Einstein. Indeed, the modern understanding of the earliest phase of quantum theory is that it was Einstein rather than Planck who, during the period 1900–1905, clearly realized that Planck’s radiation law marked a break with classical physics [Büttner *et al.*, 2003]. This insight, then, led Einstein to the quantization of energy. This he did in a twofold way, both in connection with Planck’s resonators — interpreted by Einstein as harmonic oscillators in the modern way — and, in a closely related move, through his concept of a photon. Although Planck of course introduced the constant named after him, and as such is the founding *father* of the theory characterized by  $\hbar$ , it is the introduction of the photon that made Einstein at least the *mother* of quantum theory. Einstein himself may well have regarded the photon as his most revolutionary discovery, for what he wrote about his pertinent paper is not matched in self-confidence by anything he said about relativity: ‘Sie handelt über die Strahlung und die energetischen Eigenschaften des Lichtes und ist sehr revolutionär.’<sup>21</sup>

Finally, in the light of the present paper, it deserves to be mentioned that Einstein [1905] and Planck [1906] were the first to comment on the classical limit of quantum theory; see the preamble to Section 5 below.

## 2.2 Bohr

Bohr’s brilliant model of the atom reinforced his idea that quantum theory was a theory of quanta.<sup>22</sup> Since this model simultaneously highlighted the clash between classical and quantum physics *and* carried the germ of a resolution of this conflict through Bohr’s equally brilliant correspondence principle, it is worth saying a few words about it here.<sup>23</sup> Bohr’s atomic model addressed the radiative instability of Rutherford’s solar-system-style atom:<sup>24</sup> according to the electrodynamics of Lorentz, an accelerating electron should radiate, and since the envisaged circular or elliptical motion of an electron around the nucleus is a special case of an accelerated motion, the electron should continuously lose energy and spiral towards

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<sup>21</sup>‘[This paper] is about radiation and the energetic properties of light, and is very revolutionary.’ See also the Preface to Pais [1982].

<sup>22</sup>Although at the time Bohr followed practically all physicists in their rejection of Einstein’s photon, since he believed that during a quantum jump the atom emits electromagnetic radiation in the form of a spherical wave. His model probably would have gained in consistency by adopting the photon picture of radiation, but in fact Bohr was to be the last prominent opponent of the photon, resisting the idea until 1925. See also Blair Bolles [2004] and footnote 33 below.

<sup>23</sup>Cf. [Darrigol, 1992] for a detailed treatment; also see [Liboff, 1984] and [Steiner, 1998].

<sup>24</sup>The solar system provides the popular visualization of Rutherford’s atom, but his own picture was more akin to Saturn’s rings than to a planet orbiting the Sun.



the nucleus.<sup>25</sup> Bohr countered this instability by three simultaneous moves, each of striking originality:

1. He introduced a quantization condition that singled out only a discrete number of allowed electronic orbits (which subsequently were to be described using classical mechanics, for example, in Bohr's calculation of the Rydberg constant  $R$ ).
2. He replaced the emission of continuous radiation called for by Lorentz by quantum jumps with unpredictable destinations taking place at unpredictable moments, during which the atom emits light with energy equal to the energy difference of the orbits between which the electron jumps.
3. He prevented the collapse of the atom through such quantum jumps by introducing the notion of a ground state, below which no electron could fall.

With these postulates, for which at the time there existed no foundation whatsoever,<sup>26</sup> Bohr explained the spectrum of the hydrogen atom, including an amazingly accurate calculation of  $R$ . Moreover, he proposed what was destined to be the key guiding principle in the search for quantum mechanics in the coming decade, viz. the correspondence principle (cf. [Darrigol, 1992, *passim*], and [Mehra and Rechenberg, 1982a, 249–257]).

In general, there is no relation between the energy that an electron loses during a particular quantum jump and the energy it would have radiated classically (i.e. according to Lorentz) in the orbit it revolves around preceding this jump. Indeed, in the ground state it cannot radiate through quantum jumps at all, whereas according to classical electrodynamics it should radiate all the time. However, Bohr saw that in the opposite case of very wide orbits (i.e. those having very large principal quantum numbers  $n$ ), the frequency  $\nu = (E_n - E_{n-1})/h$  (with  $E_n = -R/n^2$ ) of the emitted radiation approximately corresponds to the frequency of the lowest harmonic of the classical theory, applied to electron motion in the initial orbit.<sup>27</sup> Moreover, the measured intensity of the associated spectral line (which theoretically should be related to the probability of the quantum jump, a quantity out of the reach of early quantum theory), similarly turned out to be given by classical electrodynamics. This property, which in simple cases could be verified either by explicit computation or by experiment, became a guiding principle in situations where it could not be verified, and was sometimes even

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<sup>25</sup>In addition, any Rutherford style atom with more than one electron is mechanically unstable, since the electrons repel each other, as opposed to planets, which attract each other.

<sup>26</sup>What has hitherto been mathematically proved of Bohr's atomic model is the existence of a ground state (see [Griesemer *et al.*, 2001], and references therein for the greatest generality available to date) and the metastability of the excited states of the atom after coupling to the electromagnetic field (cf. [Bach *et al.*, 1998; 1999] and [Gustafson and Sigal, 2003]). The energy spectrum is discrete only if the radiation field is decoupled, leading to the usual computation of the spectrum of the hydrogen atom first performed by Schrödinger and Weyl. See also the end of Subsection 5.4.

<sup>27</sup>Similarly, higher harmonics correspond to quantum jumps  $n \rightarrow n - k$  for  $k > 1$ .

extended to low quantum numbers, especially when the classical theory predicted selection rules.

It should be emphasized that *Bohr's correspondence principle was concerned with the properties of radiation, rather than with the mechanical orbits themselves*.<sup>28</sup> This is not quite the same as what is usually called the correspondence principle in the modern literature.<sup>29</sup> In fact, although also this modern correspondence principle has a certain range of validity (as we shall see in detail in Section 5), Bohr never endorsed anything like that, and is even on record as opposing such a principle:<sup>30</sup>

‘The place was Purcell’s office where Purcell and others had taken Bohr for a few minutes of rest [during a visit to the Physics Department at Harvard University in 1961]. They were in the midst of a general discussion when Bohr commented: “People say that classical mechanics is the limit of quantum mechanics when  $h$  goes to zero.” Then, Purcell recalled, Bohr shook his finger and walked to the blackboard on which he wrote  $e^2/hc$ . As he made three strokes under  $h$ , Bohr turned around and said, “you see  $h$  is in the denominator.”’

### 2.3 Heisenberg

Heisenberg’s [1925] paper *Über die quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen*<sup>31</sup> is generally seen as a turning point in the development of quantum mechanics. Even A. Pais, no friend of Heisenberg’s,<sup>32</sup> conceded that Heisenberg’s paper marked ‘one of the great jumps — perhaps the greatest — in the development of twentieth century physics.’ What did Heisenberg actually accomplish? This question is particularly interesting from the perspective of our theme.

At the time, atomic physics was in a state of crisis, to which various camps responded in different ways. Bohr’s approach might best be described as *damage control*: his quantum theory was a hybrid of classical mechanics adjusted by means of *ad hoc* quantization rules, whilst keeping electrodynamics classical at all cost.<sup>33</sup>

<sup>28</sup>As such, it remains to be verified in a rigorous way.

<sup>29</sup>A typical example of the modern version is: ‘Non-relativistic quantum mechanics was founded on the correspondence principle of Bohr: “When the Planck constant  $\hbar$  can be considered small with respect to the other parameters such as masses and distances, quantum theory approaches classical Newton theory.”’ [Robert, 1998, 44]. The reference to Bohr is historically inaccurate!

<sup>30</sup>Quoted from [Miller, 1984, 313].

<sup>31</sup>*On the quantum theoretical reinterpretation of kinematical and mechanical relations*. English translation in [van der Waerden, 1967].

<sup>32</sup>For example, in [Pais, 2000], claiming to portray the ‘genius of science’, Heisenberg is conspicuously absent.

<sup>33</sup>Continuing footnote 22, we quote from [Mehra and Rechenberg, 1982a, 256–257]: ‘Thus, in the early 1920s, Niels Bohr arrived at a definite point of view how to proceed forward in atomic theory. He wanted to make maximum use of what he called the “more dualistic prescription” (...) In it the atom was regarded as a mechanical system having discrete states and emitting radiation of discrete frequencies, determined (in a nonclassical way) by the energy differences

Einstein, who had been the first physicist to recognize the need to quantize classical electrodynamics, in the light of his triumph with General Relativity nonetheless dreamt of a classical field theory with singular solutions as the ultimate explanation of quantum phenomena. Born led the radical camp, which included Pauli: he saw the need for an entirely new mechanics replacing classical mechanics,<sup>34</sup> which was to be based on discrete quantities satisfying difference equations.<sup>35</sup> This was a leap in the dark, especially because of Pauli's frowning upon the correspondence principle [Hendry, 1984; Beller, 1999].

It was Heisenberg's genius to *interpolate* between Bohr and Born.<sup>36</sup> The meaning of his *Umdeutung* was to keep the classical equations of motion,<sup>37</sup> whilst reinterpreting the mathematical symbols occurring therein as (what were later recognized to be) matrices. Thus his *Umdeutung*  $x \mapsto a(n, m)$  was a precursor of what now would be called a quantization map  $f \mapsto Q_{\hbar}(f)$ , where  $f$  is a classical observable, i.e. a function on phase space, and  $Q_{\hbar}(f)$  is a quantum mechanical observable, in the sense of an operator on a Hilbert space or, more abstractly, an element of some  $C^*$ -algebra. See Section 4 below. As Heisenberg recognized, this move implies the noncommutativity of the quantum mechanical observables; it is this, rather than something like a "quantum postulate" (see Subsection 3.2 below), that is the defining characteristic of quantum mechanics. Indeed, most later work on quantum physics and practically all considerations on the connection between classical and quantum rely on Heisenberg's idea of *Umdeutung*. This even applies to the mathematical formalism as a whole; see Subsection 2.5.

We here use the term "observable" in a loose way. It is now well recognized [Mehra and Rechenberg, 1982b; Beller, 1999; Camilleri, 2005] that Heisenberg's claim that his formalism could be physically interpreted as the replacement of atomic orbits by observable quantities was a red herring, inspired by his discussions with Pauli. In fact, in quantum mechanics *any* mechanical quantity has to be "reinterpreted", whether or not it is observable. As Heisenberg [1969] recalls, Einstein reprimanded him for the illusion that physics admits an *a priori* notion of an observable, and explained that a theory determines what can be observed. Rethinking the issue of observability then led Heisenberg to his second major contribution to quantum mechanics, namely his uncertainty relations.

These relations were Heisenberg's own answer to the quote opening this paper. Indeed, matrix mechanics was initially an extremely abstract and formal scheme,

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between stationary states; radiation, on the other hand, had to be described by the classical electrodynamic theory.<sup>7</sup>

<sup>34</sup>It was Born who coined the name *quantum mechanics* even before Heisenberg's paper.

<sup>35</sup>This idea had earlier occurred to Kramers.

<sup>36</sup>Also literally! Heisenberg's traveled between Copenhagen and Göttingen most of the time.

<sup>37</sup>This crucial aspect of *Umdeutung* was appreciated at once by Dirac [1926]: 'In a recent paper Heisenberg puts forward a new theory which suggests that it is not the equations of classical mechanics that are in any way at fault, but that the mathematical operations by which physical results are deduced from them require modification. (...) The correspondence between the quantum and classical theories lies not so much in the limiting agreement when  $\hbar \rightarrow 0$  as in the fact that the mathematical operations on the two theories obey in many cases the same laws.'

which lacked not only any visualization but also the concept of a state (see below). Although these features were initially quite to the liking of Born, Heisenberg, Pauli, and Jordan, the success of Schrödinger's work forced them to renege on their radical stance, and look for a semiclassical picture supporting their mathematics; this was a considerable U-turn [Beller, 1999; Camilleri, 2005]. Heisenberg [1927] found such a picture, claiming that his uncertainty relations provided the 'intuitive content of the quantum theoretical kinematics and mechanics' (as his paper was called). His idea was that *the classical world emerged from quantum mechanics through observation*: 'The trajectory only comes into existence because we observe it.'<sup>38</sup> This idea was to become extremely influential, and could be regarded as the origin of stance 1 in the Introduction.

## 2.4 Schrödinger

The history of quantum mechanics is considerably clarified by the insight that Heisenberg and Schrödinger did not, as is generally believed, discover two equivalent formulations of the theory, but rather that Heisenberg [1925] identified the mathematical nature of the observables, whereas Schrödinger [1926a] found the description of states.<sup>39</sup> Matrix mechanics lacked the notion of a state, but by the same token wave mechanics initially had no observables; it was only in his attempts to relate wave mechanics to matrix mechanics that Schrödinger [1926c] introduced the position and momentum operators<sup>40</sup>

$$\begin{aligned} \mathcal{Q}_{\hbar}(q^j) &= x^j; \\ (2) \quad \mathcal{Q}_{\hbar}(p_j) &= -i\hbar \frac{\partial}{\partial x^j}. \end{aligned}$$

This provided a new basis for Schrödinger's equation<sup>41</sup>

$$(3) \quad \left( -\frac{\hbar^2}{2m} \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2} + V(x) \right) \Psi = i\hbar \frac{\partial \Psi}{\partial t},$$

by interpreting the left-hand side as  $H\Psi$ , with  $H = \mathcal{Q}_{\hbar}(h)$  in terms of the classical Hamiltonian  $h(p, q) = \sum_j p_j^2/2m + V(q)$ . Thus Schrödinger founded the theory of the operators now named after him,<sup>42</sup> and in doing so gave what is still the most important example of Heisenberg's idea of *Umdeutung* of classical observables.

<sup>38</sup>'Die Bahn entsteht erst dadurch, daß wir sie beobachten.'

<sup>39</sup>See also [Muller, 1997].

<sup>40</sup>Here  $j = 1, 2, 3$ . In modern terms, the expressions on the right-hand side are unbounded operators on the Hilbert space  $\mathcal{H} = L^2(\mathbb{R}^n)$ . See Section 4 for more details. The expression  $x^j$  is a multiplication operator, i.e.  $(x^j\Psi)(x) = x^j\Psi(x)$ , whereas, obviously,  $(\partial/\partial x^j\Psi)(x) = (\partial\Psi/\partial x^j)(x)$ .

<sup>41</sup>Or the corresponding time-independent one, with  $E\Psi$  on the right-hand side.

<sup>42</sup>See [Reed and Simon, 1972; 1975; 1987; 1979; Cycon *et al.*, 1987; Hislop and Sigal, 1996; Hunziker and Sigal, 2000; Simon, 2000; Gustafson and Sigal, 2003]. For the mathematical origin of the Schrödinger equation also cf. [Simon, 1976].

Subsequently, correcting and expanding on certain ideas of Dirac, Pauli, and Schrödinger, von Neumann [1932] brilliantly glued these two parts together through the concept of a Hilbert space. He also gave an abstract form of the formulae of Born, Pauli, Dirac, and Jordan for the transition probabilities, thus completing the mathematical formulation of quantum mechanics.

However, this is not how Schrödinger saw his contribution. He intended wave mechanics as a full-fledged classical field theory of reality, rather than merely as one half (namely in modern parlance the state space half) of a probabilistic description of the world that still incorporated the quantum jumps he so detested [Mehra and Rechenberg, 1987; Götsch, 1992; Bitbol and Darrigol, 1992; Bitbol, 1996; Beller, 1999]. Particles were supposed to emerge in the form of wave packets, but it was immediately pointed out by Heisenberg, Lorentz, and others that in realistic situations such wave packets tend to spread in the course of time. This had initially been overlooked by Schrödinger [1926b], who had based his intuition on the special case of the harmonic oscillator. On the positive side, in the course of his unsuccessful attempts to derive classical particle mechanics from wave mechanics through the use of wave packets, Schrödinger [1926b] gave the first example of what is now called a *coherent state*. Here a quantum wave function  $\Psi_z$  is labeled by a ‘classical’ parameter  $z$ , in such a way that the quantum-mechanical time-evolution  $\Psi_z(t)$  is approximately given by  $\Psi_{z(t)}$ , where  $z(t)$  stands for some associated classical time-evolution; see Subsections 4.2 and 5.2 below. This has turned out to be a very important idea in understanding the transition from quantum to classical mechanics.

Furthermore, in the same paper Schrödinger [1926b] proposed the following wave-mechanical version of Bohr’s correspondence principle: classical atomic states should come from superpositions of a very large number (say at least 10,000) of highly excited states (i.e. energy eigenfunctions with very large quantum numbers). After decades of limited theoretical interest in this idea, interest in wave packets in atomic physics was revived in the late 1980s due to the development of modern experimental techniques based on lasers (such as pump-probing and phase-modulation). See [Robinett, 2004] for a recent technical review, or [Nauenberg *et al.*, 1994] for an earlier popular account. Roughly speaking, the picture that has emerged is this: a localized wave packet of the said type initially follows a time-evolution with almost classical periodicity, as Schrödinger hoped, but subsequently spreads out after a number of orbits. Consequently, during this second phase the probability distribution approximately fills the classical orbit (though not uniformly). Even more surprisingly, on a much longer time scale there is a phenomenon of *wave packet revival*, in which the wave packet recovers its initial localization. Then the whole cycle starts once again, so that one does see periodic behaviour, but not of the expected classical type. Hence even in what naively would be thought of as the thoroughly classical regime, wave phenomena continue to play a role, leading to quite unusual and unexpected behaviour. Although a rigorous mathematical description of wave packet revival has not yet been forthcoming, the overall picture (based on both “theoretical physics” style mathematics

and experiments) is clear enough.

It is debatable (and irrelevant) whether the story of wave packets has evolved according to Schrödinger's intentions (cf. [Littlejohn, 1986]); what is certain is that his other main idea on the relationship between classical and quantum has been extremely influential. This was, of course, Schrödinger's [1926a] "derivation" of his wave equation from the Hamilton–Jacobi formalism of classical mechanics. This gave rise to the WKB approximation and related methods; see Subsection 5.5.

In any case, where Schrödinger hoped for a classical interpretation of his wave function, and Heisenberg wanted to have nothing to do with it whatsoever [Beller, 1999], Born and Pauli were quick to realize its correct, probabilistic significance. Thus they deprived the wave function of its naive physical nature, and effectively degraded it to the purely mathematical status of a probability amplitude. And in doing so, Born and Pauli rendered the connection between quantum mechanics and classical mechanics almost incomprehensible once again! It was this incomprehensibility that Heisenberg addressed with his uncertainty relations.

## 2.5 von Neumann

Through its creation of the Hilbert space formalism of quantum mechanics, von Neumann's book [1932] can be seen as a mathematical implementation of Heisenberg's idea of *Umdeutung*. Von Neumann in effect proposed the following quantum-theoretical reinterpretations:

Phase space  $M \mapsto$  Hilbert space  $\mathcal{H}$ ;

Classical observable (i.e. real-valued measurable function on  $M$ )  $\mapsto$  self-adjoint operator on  $\mathcal{H}$ ;

Pure state (seen as point in  $M$ )  $\mapsto$  unit vector (actually ray) in  $\mathcal{H}$ ;

Mixed state (i.e. probability measure on  $M$ )  $\mapsto$  density matrix on  $\mathcal{H}$ ;

Measurable subset of  $M \mapsto$  closed linear subspace of  $\mathcal{H}$ ;

Set complement  $\mapsto$  orthogonal complement;

Union of subsets  $\mapsto$  closed linear span of subspaces;

Intersection of subsets  $\mapsto$  intersection of subspaces;

Yes-no question (i.e. characteristic function on  $M$ )  $\mapsto$  projection operator.<sup>43</sup>

Here we assume for simplicity that quantum observables  $R$  on a Hilbert space  $\mathcal{H}$  are bounded operators, i.e.  $R \in \mathcal{B}(\mathcal{H})$ . Von Neumann actually *derived* his *Umdeutung* of classical mixed states as density matrices from his axiomatic characterization of quantum-mechanical states as linear maps  $\text{Exp} : \mathcal{B}(\mathcal{H}) \rightarrow \mathbb{C}$  that

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<sup>43</sup>Later on, he of course added the *Umdeutung* of a Boolean lattice by a modular lattice, and the ensuing *Umdeutung* of classical logic by quantum logic [Birkhoff and von Neumann, 1936].

satisfy  $\text{Exp}(R) \geq 0$  when  $R \geq 0$ ,<sup>44</sup>  $\text{Exp}(1) = 1$ ,<sup>45</sup> and countable additivity on a commuting set of operators. For he proved that such a map  $\text{Exp}$  is necessarily given by a density matrix  $\rho$  according to  $\text{Exp}(R) = \text{Tr}(\rho R)$ .<sup>46</sup> A unit vector  $\Psi \in \mathcal{H}$  defines a pure state in the sense of von Neumann, which we call  $\psi$ , by  $\psi(R) = (\Psi, R\Psi)$  for  $R \in \mathcal{B}(\mathcal{H})$ . Similarly, a density matrix  $\rho$  on  $\mathcal{H}$  defines a (generally mixed) state, called  $\rho$  as well, by  $\rho(R) = \text{Tr}(\rho R)$ . In modern terminology, a state on  $\mathcal{B}(\mathcal{H})$  as defined by von Neumann would be called a *normal* state. In the  $C^*$ -algebraic formulation of quantum physics (cf. footnote 7), this axiomatization has been maintained until the present day; here  $\mathcal{B}(\mathcal{H})$  is replaced by more general algebras of observables in order to accommodate possible superselection rules [Haag, 1992].

Beyond his mathematical axiomatization of quantum mechanics, which (along with its subsequent extension by the  $C^*$ -algebraic formulation) lies at the basis of all serious efforts to relate classical and quantum mechanics, von Neumann contributed to this relationship through his analysis of the measurement problem.<sup>47</sup> Since here the apparent clash between classical and quantum physics comes to a head, it is worth summarizing von Neumann's analysis of this problem here. See also [Wheeler and Zurek, 1983; Busch *et al.*, 1991; Auletta, 2001] and [Mittelstaedt, 2004] for general discussions of the measurement problem.

The essence of the measurement problem is that certain states are never seen in nature, although they are not merely allowed by quantum mechanics (on the assumption of its universal validity), but are even predicted to arise in typical measurement situations. Consider a system  $S$ , whose pure states are mathematically described by normalized vectors (more precisely, rays) in a Hilbert space  $\mathcal{H}_S$ . One wants to measure an observable  $\mathcal{O}$ , which is mathematically represented by a self-adjoint operator  $O$  on  $\mathcal{H}_S$ . Von Neumann assumes that  $O$  has discrete

<sup>44</sup>I.e., when  $R$  is self-adjoint with positive spectrum, or, equivalently, when  $R = S^*S$  for some  $S \in \mathcal{B}(\mathcal{H})$ .

<sup>45</sup>Where the 1 in  $\text{Exp}(1)$  is the unit operator on  $\mathcal{H}$ .

<sup>46</sup>This result has been widely misinterpreted (apparently also by von Neumann himself) as a theorem excluding hidden variables in quantum mechanics. See [Scheibe, 1991]. However, Bell's characterization of von Neumann's linearity assumption in the definition of a state as "silly" is far off the mark, since it holds both in classical mechanics and in quantum mechanics. Indeed, von Neumann's theorem *does* exclude all hidden variable extensions of quantum mechanics that are classical in nature, and it is precisely such extensions that many physicists were originally looking for. See [Rédei and Stöltzner, 2001] and [Scheibe, 2001] for recent discussions of this issue.

<sup>47</sup>Von Neumann [1932] refrained from discussing either the classical limit of quantum mechanics or (probably) the notion of quantization. In the latter direction, he declares that 'If the quantity  $\mathfrak{R}$  has the operator  $R$ , then the quantity  $f(\mathfrak{R})$  has the operator  $f(R)$ ', and that 'If the quantities  $\mathfrak{R}, \mathfrak{S}, \dots$  have the operators  $R, S, \dots$ , then the quantity  $\mathfrak{R} + \mathfrak{S} + \dots$  has the operator  $R + S + \dots$ '. However, despite his legendary clarity and precision, von Neumann is rather vague about the meaning of the transition  $\mathfrak{R} \mapsto R$ . It is tempting to construe  $\mathfrak{R}$  as a classical observable whose quantum-mechanical counterpart is  $R$ , so that the above quotations might be taken as axioms for quantization. However, such an interpretation is neither supported by the surrounding text, nor by our current understanding of quantization (cf. Section 4). For example, a quantization map  $\mathfrak{R} \mapsto \mathcal{Q}_\hbar(\mathfrak{R})$  cannot satisfy  $f(\mathfrak{R}) \mapsto f(\mathcal{Q}_\hbar(\mathfrak{R}))$  even for very reasonable functions such as  $f(x) = x^2$ .

spectrum, a simplification which does not hide the basic issues in the measurement problem. Hence  $O$  has unit eigenvectors  $\Psi_n$  with real eigenvalues  $o_n$ . To measure  $O$ , one couples the system to an apparatus  $A$  with Hilbert space  $\mathcal{H}_A$  and “pointer” observable  $\mathcal{P}$ , represented by a self-adjoint operator  $P$  on  $\mathcal{H}_A$ , with discrete eigenvalues  $p_n$  and unit eigenvectors  $\Phi_n$ . The pure states of the total system  $S + A$  then correspond to unit vectors in the tensor product  $\mathcal{H}_S \otimes \mathcal{H}_A$ . A good (“first kind”) measurement is then such that after the measurement,  $\Psi_n$  is correlated to  $\Phi_n$ , that is, for a suitably chosen initial state  $I \in \mathcal{H}_A$ , a state  $\Psi_n \otimes I$  (at  $t = 0$ ) almost immediately evolves into  $\Psi_n \otimes \Phi_n$ . This can indeed be achieved by a suitable Hamiltonian.

The problem, highlighted by Schrödinger’s cat, now arises if one selects the initial state of  $S$  to be  $\sum_n c_n \Psi_n$  (with  $\sum |c_n|^2 = 1$ ), for then the superposition principle leads to the conclusion that the final state of the coupled system is  $\sum_n c_n \Psi_n \otimes \Phi_n$ . Now, basically all von Neumann said was that if one restricts the final state to the system  $S$ , then the resulting density matrix is the mixture  $\sum_n |c_n|^2 [\Psi_n]$  (where  $[\Psi]$  is the orthogonal projection onto a unit vector  $\Psi$ ),<sup>48</sup> so that, *from the perspective of the system alone*, the measurement appears to have caused a transition from the pure state  $\sum_{n,m} c_n \bar{c}_m \Psi_n \Psi_m^*$  to the mixed state  $\sum_n |c_n|^2 [\Psi_n]$ , in which interference terms  $\Psi_n \Psi_m^*$  for  $n \neq m$  are absent. Here the operator  $\Psi_n \Psi_m^*$  is defined by  $\Psi_n \Psi_m^* f = (\Psi_m, f) \Psi_n$ ; in particular,  $\Psi \Psi^* = [\Psi]$ .<sup>49</sup> Similarly, the apparatus, taken by itself, has evolved from the pure state  $\sum_{n,m} c_n \bar{c}_m \Phi_n \Phi_m^*$  to the mixed state  $\sum_n |c_n|^2 [\Phi_n]$ . This is simply a mathematical theorem (granted the possibility of coupling the system to the apparatus in the desired way), rather than a proposal that there exist two different time-evolutions in Nature, viz. the unitary propagation according to the Schrödinger equation side by side with the above “collapse” process.

In any case, by itself this move by no means solves the measurement problem.<sup>50</sup> Firstly, in the given circumstances one is not allowed to adopt the ignorance interpretation of mixed states (i.e. assume that the system really is in one of the states  $\Psi_n$ ); cf., e.g., [Mittelstaedt, 2004]. Secondly, even if one were allowed to do so, one could restore the problem (i.e. the original superposition  $\sum_n c_n \Psi_n \otimes \Phi_n$ ) by once again taking the other component of the system into account.

Von Neumann was well aware of at least this second point, to which he responded by his construction of a *chain*: one redefines  $S + A$  as the system, and couples it to a new apparatus  $B$ , etc. This eventually leads to a post-measurement state  $\sum_n c_n \Psi_n \otimes \Phi_n \otimes \chi_n$  (in hopefully self-explanatory notation, assuming the vectors  $\chi_n$  form an orthonormal set), whose restriction to  $S + A$  is the mixed state  $\sum_n |c_n|^2 [\Psi_n] \otimes [\Phi_n]$ . The restriction of the latter state to  $S$  is, once again,  $\sum_n |c_n|^2 [\Psi_n]$ . This procedure may evidently be iterated; the point of the construction is evidently to pass on superpositions in some given system to arbitrary

<sup>48</sup>I.e.,  $[\Psi]f = (\Psi, f)\Psi$ ; in Dirac notation one would have  $[\Psi] = |\Psi\rangle\langle\Psi|$ .

<sup>49</sup>In Dirac notation one would have  $\Psi_n \Psi_m^* = |\Psi_n\rangle\langle\Psi_m|$ .

<sup>50</sup>Not even in an ensemble-interpretation of quantum mechanics, which was the interpretation von Neumann unfortunately adhered to when he wrote his book.



systems higher up in the chain. It follows that for the final state of the original system it does not matter where one “cuts the chain” (that is, which part of the chain one leaves out of consideration), as long as it is done *somewhere*. Von Neumann ([1932], in beautiful prose) and others suggested identifying the cutting with the act of observation, but it is preferable and much more general to simply say that *some* end of the chain is omitted in the description.

The burden of the measurement problem, then, is to

1. Construct a suitable chain along with an appropriate cut thereof; it doesn't matter where the cut is made, as long as it is done.
2. Construct a suitable time-evolution accomplishing the measurement.
3. Justify the ignorance interpretation of mixed states.

As we shall see, these problems are addressed, in a conceptually different but mathematically analogous way, in the Copenhagen interpretation as well as in the decoherence approach. (The main conceptual difference will be that the latter aims to solve also the more ambitious problem of explaining the appearance of the classical world, which in the former seems to be taken for granted).

We conclude this section by saying that despite some brilliant ideas, the founders of quantum mechanics left wide open the problem of deriving classical mechanics as a certain regime of their theory.

### 3 COPENHAGEN: A REAPPRAISAL

The so-called “Copenhagen interpretation” of quantum mechanics goes back to ideas first discussed and formulated by Bohr, Heisenberg, and Pauli around 1927. Against the idea that there has been a “party line” from the very beginning, it has frequently been pointed out that in the late 1920s there were actually sharp differences of opinion between Bohr and Heisenberg on the interpretation of quantum mechanics and that they never really arrived at a joint doctrine [Hooker, 1972; Stapp, 1972; Hendry, 1984; Beller, 1999; Howard, 2004; Camilleri, 2005]. For example, they never came to agree about the notion of complementarity (see Subsection 3.3). More generally, Heisenberg usually based his ideas on the mathematical formalism of quantum theory, whereas Bohr's position was primarily philosophically oriented. Nonetheless, there is a clearly identifiable core of ideas on which they *did* agree, and since this core has everything to do with the relationship between classical and quantum, we are going to discuss it in some detail.

The principal primary sources are Bohr's Como Lecture, his reply to EPR, and his essay dedicated to Einstein [Bohr, 1927; 1935; 1949].<sup>51</sup> Historical discussions of the emergence and reception of these papers are given in Bohr [1985; 1996] and in Mehra and Rechenberg [2001]. As a selection of the enormous literature

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<sup>51</sup>These papers were actually written in collaboration with Pauli (after first attempts with Klein), Rosenfeld, and Pais, respectively.

these papers have given rise to, we mention among relatively recent works [Hooker, 1972; Scheibe, 1973; Folse, 1985; Murdoch, 1987; Lahti and Mittelstaedt, 1987; Honner, 1987; Chevalley, 1991; 1999; Faye, 1991; Faye and Folse, 1994; Held, 1994; Howard, 1994; Beller, 1999; Faye, 2002], and [Saunders, 2005]. For Bohr's sparring partners see [Heisenberg, 1930; 1942; 1958; 1984a,b; 1985] with associated secondary literature [Heelan, 1965; Hörz, 1968; Geyer *et al.*, 1993; Camilleri, 2005] and [Pauli, 1933; 1949; 1979; 1985; 1994]), along with [Laurikainen, 1988] and [Enz, 2002].

As with Wittgenstein (and many other thinkers), it helps to understand Bohr if one makes a distinction between an “early” Bohr and a “later” Bohr.<sup>52</sup> Despite a good deal of continuity in his thought (see below), the demarcation point is his response to EPR [Bohr, 1935],<sup>53</sup> and the main shift he made afterwards lies in his sharp insistence on the indivisible unity of object and observer after 1935, focusing on the concept of a *phenomenon*. Before EPR, Bohr equally well believed that object and observer were both necessary ingredients of a complete description of quantum theory, but he then thought that although their interaction could never be neglected, they might at least logically be considered separately. After 1935, Bohr gradually began to claim that object and observer no longer even had separate identities, together forming a “phenomenon”. Accordingly, also his notion of complementarity changed, increasingly focusing on the idea that the specification of the experimental conditions is crucial for the unambiguous use of (necessarily) classical concepts in quantum theory [Scheibe, 1973; Held, 1994]. See also Subsection 3.3 below. This development culminated in Bohr's eventual denial of the existence of the quantum world:

‘There is no quantum world. There is only an abstract quantum-physical description. It is wrong to think that the task of physics is to find out how nature is. Physics concerns what we can say about nature. (...) What is it that we humans depend on? We depend on our words. Our task is to communicate experience and ideas to others. We are suspended in language.’ (quoted by [Petersen, 1963, 8].)<sup>54</sup>

### 3.1 *The doctrine of classical concepts*

Despite this shift, it seems that Bohr stuck to one key thought throughout his career:

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<sup>52</sup>Here we side with Held [1994] and Beller [1999] against Howard [1994] and Saunders [2005]. See also [Pais, 2000, 22]: ‘Bohr's Como Lecture did not bring the house down, however. He himself would later frown on expressions he used there, such as “disturbing the phenomena by observation”. Such language may have contributed to the considerable confusion that for so long has reigned around this subject.’

<sup>53</sup>This response is problematic, as is EPR itself. Consequently, there exists a considerable exegetical literature on both, marked by the fact that equally competent and well-informed pairs of commentators manage to flatly contradict each other while at the same time both claiming to explain or reconstruct what Bohr “really” meant.

<sup>54</sup>See [Mermin, 2004] for a witty discussion of this controversial quotation.

‘However far the phenomena transcend the scope of classical physical explanation, the account of all evidence must be expressed in classical terms. (...) The argument is simply that by the word *experiment* we refer to a situation where we can tell others what we have done and what we have learned and that, therefore, the account of the experimental arrangements and of the results of the observations must be expressed in unambiguous language with suitable application of the terminology of classical physics.’ [Bohr, 1949, 209].

This is, in a nutshell, Bohr’s *doctrine of classical concepts*. Although his many drawings and stories may suggest otherwise, Bohr does not quite express the idea here that the goal of physics lies in the description of experiments.<sup>55</sup> In fact, he merely points out the need for “unambiguous” communication, which he evidently felt threatened by quantum mechanics.<sup>56</sup> The controversial part of the quote lies in his identification of the means of unambiguous communication with the language of classical physics, involving particles and waves and the like. We will study Bohr’s specific argument in favour of this identification shortly, but it has to be said that, like practically all his foundational remarks on quantum mechanics, Bohr presents his reasoning as self-evident, necessary, and not in need of any further analysis [Scheibe, 1973; Beller, 1999]. Nonetheless, young Heisenberg clashed with Bohr on precisely this point, for Heisenberg felt that the abstract mathematical formalism of quantum theory (rather than Bohr’s world of words and pictures) provided those means of unambiguous communication.<sup>57</sup>

By classical physics Bohr undoubtedly meant the theories of Newton, Maxwell, and Lorentz, but that is not the main point.<sup>58</sup> For Bohr, the *defining* property of classical physics was the property that it was *objective*, i.e. that it could be studied in an observer-independent way:

‘All description of experiences so far has been based on the assumption, already inherent in ordinary conventions of language, that it is possible to distinguish sharply between the behaviour of objects and the means of observation. This assumption is not only fully justified by everyday experience, *but even constitutes the whole basis of classical physics*’

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<sup>55</sup>Which often but misleadingly has been contrasted with Einstein’s belief that the goal of physics is rather to describe reality. See [Landsman, 2006b] for a recent discussion.

<sup>56</sup>Here “unambiguous” means “objective” [Scheibe, 1973; Chevalley, 1991].

<sup>57</sup>It is hard to disagree with Beller’s [1999] conclusion that Bohr was simply not capable of understanding the formalism of post-1925 quantum mechanics, turning his own need of understanding this theory in terms of words and pictures into a deep philosophical necessity.

<sup>58</sup>Otherwise, one should wonder why one shouldn’t use the physics of Aristotle and the scholastics for this purpose, which is a much more effective way of communicating our naive impressions of the world. In contrast, the essence of physics since Newton has been to unmask a reality behind the phenomena. Indeed, Newton himself emphasized that his physics was intended for those capable of natural philosophy, in contrast to *ye vulgar* who believed naive appearances. The fact that Aristotle’s physics is now known to be wrong should not suffice to disqualify its use for Bohr’s purposes, since the very same comment may be made about the physics of Newton etc.

[Bohr, 1958, 25; italics added].<sup>59</sup>

See also [Hooker, 1972; Scheibe, 1973] and [Howard, 1994]. Heisenberg [1958, 55] shared this view:<sup>60</sup>

‘In classical physics science started from the belief — or should one say from the illusion? — that we could describe the world or at least part of the world without any reference to ourselves. This is actually possible to a large extent. We know that the city of London exists whether we see it or not. It may be said that classical physics is just that idealization in which we can speak about parts of the world without any reference to ourselves. Its success has led to the general idea of an objective description of the world.’

On the basis of his “quantum postulate” (see Subsection 3.2), Bohr came to believe that, similarly, the *defining* property of quantum physics was precisely the opposite, i.e. the necessity of the role of the observer (or apparatus — Bohr did not distinguish between the two and never assigned a special role to the mind of the observer or endorsed a subjective view of physics). Identifying unambiguous communication with an objective description, in turn claimed to be the essence of classical physics, Bohr concluded that despite itself quantum physics had to be described entirely in terms of classical physics. Thus his doctrine of classical concepts has an epistemological origin, arising from an analysis of the conditions for human knowledge.<sup>61</sup> In that sense it may be said to be Kantian in spirit [Hooker, 1972; Murdoch, 1987; Chevalley, 1991; 1999].

Now, Bohr himself is on record as saying: ‘They do it smartly, but what counts is to do it right’ [Rosenfeld, 1967, 129].<sup>62</sup> The doctrine of classical concepts is certainly smart, but is it right? As we have seen, Bohr’s argument starts from the claim that classical physics is objective (or ‘unambiguous’) in being independent of the observer. In fact, nowadays it is widely believed that quantum mechanics leads to the *opposite* conclusion that “quantum reality” (whatever that may be) is objective (though “veiled” in the terminology of d’Espagnat [1995]), while “classical reality” only comes into existence relative to a certain specification: this is

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<sup>59</sup>Despite the typical imperative tone of this quotation, Bohr often regarded certain other properties as essential to classical physics, such as determinism, the combined use of space-time concepts and dynamical conservation laws, and the possibility of pictorial descriptions. However, these properties were in some sense secondary, as Bohr considered them to be *consequences* of the possibility of isolating an object in classical physics. For example: ‘The assumption underlying the ideal of causality [is] that the behaviour of the object is uniquely determined, quite independently of whether it is observed or not’ [Bohr, 1937], and then again, now negatively: ‘the renunciation of the ideal of causality [in quantum mechanics] is founded logically only on our not being any longer in a position to speak of the autonomous behaviour of a physical object’ [Bohr, 1937]. See [Scheibe, 1973].

<sup>60</sup>As Camilleri [2005, 161] states: ‘For Heisenberg, classical physics is the fullest expression of the ideal of objectivity.’

<sup>61</sup>See, for example, the very *title* of Bohr [1958]!

<sup>62</sup>‘They’ refers to EPR.

stance 1 discussed in the Introduction.<sup>63</sup> Those who disagree with stance 1 cannot use stance 2 (of denying the fundamental nature of quantum theory) at this point either, as that is certainly not what Bohr had in mind. Unfortunately, in his most outspoken defence of Bohr, even Heisenberg [1958, 55] was unable to find a better argument for Bohr's doctrine than the lame remark that 'the use of classical concepts is finally a consequence of the general human way of thinking.'<sup>64</sup>

In our opinion, Bohr's *motivation* for his doctrine has to be revised in the light of our current understanding of quantum theory; we will do so in Subsection 3.4. In any case, whatever its motivation, the doctrine *itself* seems worth keeping: apart from the fact that it evidently describes experimental practice, it provides a convincing explanation for the probabilistic nature of quantum mechanics (cf. the next subsection).

### 3.2 *Object and apparatus: the Heisenberg cut*

Describing quantum physics in terms of classical concepts sounds like an impossible and even self-contradictory task (cf. [Heisenberg, 1958]). For one, it precludes a completely quantum-mechanical description of the world: 'However far the phenomena transcend the scope of classical physical explanation, the account of all evidence must be expressed in classical terms.' But at the same time it precludes a purely classical description of the world, for underneath classical physics one has quantum theory.<sup>65</sup> The fascination of Bohr's philosophy of quantum mechanics lies precisely in his brilliant resolution of this apparently paradoxical situation.

The first step of this resolution that he and Heisenberg proposed is to divide the system whose description is sought into two parts: one, the object, is to be described quantum-mechanically, whereas the other, the apparatus, is treated *as if it were classical*. Despite innumerable claims to the contrary in the literature (i.e. to the effect that Bohr held that a separate realm of Nature was intrinsically classical), there is no doubt that both Bohr and Heisenberg believed in the fundamental and universal nature of quantum mechanics, and saw the classical description of the apparatus as a *purely epistemological move without any coun-*

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<sup>63</sup>Indeed, interesting recent attempts to make Bohr's philosophy of quantum mechanics precise accommodate the a priori status of classical observables into some version of the modal interpretation; see [Dieks, 1989b; Bub, 1999; Halvorson and Clifton, 1999; 2002], and [Dickson, 2005]. It should give one some confidence in the possibility of world peace that the two most hostile interpretations of quantum mechanics, viz. Copenhagen and Bohm [Cushing, 1994] have now found a common home in the modal interpretation in the sense of the authors just cited! Whether or not one agrees with Bub's [2004] criticism of the modal interpretation, Bohr's insistence on the necessity of classical concepts is not vindicated by any current version of it.

<sup>64</sup>And similarly: 'We are forced to use the language of classical physics, simply because we have no other language in which to express the results.' [Heisenberg, 1971, 130]. This in spite of the fact that the later Heisenberg thought about this matter very deeply; see, e.g., his [1942], as well as [Camilleri, 2005]. Murdoch [1987, 207–210] desperately tries to boost the doctrine of classical concepts into a profound philosophical argument by appealing to Strawson [1959].

<sup>65</sup>This peculiar situation makes it very hard to give a realist account of the Copenhagen interpretation, since quantum reality is denied whereas classical reality is neither fundamental nor real.

*terpart in ontology*, expressing the fact that a given *quantum* system is *being used* as a measuring device.<sup>66</sup> For example: ‘The construction and the functioning of all apparatus like diaphragms and shutters, serving to define geometry and timing of the experimental arrangements, or photographic plates used for recording the localization of atomic objects, will depend on properties of materials which are themselves essentially determined by the quantum of action’ [Bohr, 1948, 315], as well as: ‘We are free to make the cut only within a region where the quantum mechanical description of the process concerned is effectively equivalent with the classical description’ [Bohr, 1935, 701].<sup>67</sup>

The separation between object and apparatus called for here is usually called the *Heisenberg cut*, and it plays an absolutely central role in the Copenhagen interpretation of quantum mechanics.<sup>68</sup> The idea, then, is that *a quantum-mechanical object is studied exclusively through its influence on an apparatus that is described classically*. Although *described* classically, the apparatus is a quantum system, and is supposed to be influenced by its *quantum-mechanical* coupling to the underlying (quantum) object.

The alleged necessity of including both object and apparatus in the description was initially claimed to be a consequence of the so-called “quantum postulate”. This notion played a key role in Bohr’s thinking: his Como Lecture [Bohr, 1927] was even entitled ‘The quantum postulate and the recent development of atomic theory’. There he stated its contents as follows: ‘The essence of quantum theory is the quantum postulate: every atomic process has an essential discreteness — completely foreign to classical theories — characterized by Planck’s quantum of action.’<sup>69</sup> Even more emphatically, in his reply to EPR [Bohr, 1935, 697]: ‘Indeed the finite interaction between object and measuring agencies conditioned by the

<sup>66</sup>See especially [Scheibe, 1973] on Bohr, and [Heisenberg, 1958]. The point in question has also been made by R. Haag (who knew both Bohr and Heisenberg) in most of his talks on quantum mechanics in the 1990s. In this respect we disagree with Howard [1994], who claims that according to Bohr a classical description of an apparatus amounts to picking a particular (maximally) abelian subalgebra of its quantum-mechanical algebra of ‘beables’, which choice is dictated by the measurement context. But having a commutative algebra falls far short of a classical description, since in typical examples one obtains only half of the canonical classical degrees of freedom in this way. Finding a classical description of a quantum-mechanical system is a much deeper problem, to which we shall return throughout this paper.

<sup>67</sup>This last point suggests that the cut has something to do with the division between a microscopic and a macroscopic realm in Nature, but although this division often facilitates making the cut when it is well defined, this is by no means a matter of principle. Cf. [Howard, 1994]. In particular, all objections to the Copenhagen interpretation to the effect that the interpretation is ill-defined because the micro-macro distinction is blurred are unfounded.

<sup>68</sup>Pauli [1949] went as far as saying that the Heisenberg cut provides the appropriate generalization modern physics offers of the old Kantian opposition between a knowable object and a knowing subject: ‘Auf diese Weise verallgemeinert die moderne Physik die alte Gegenüberstellung von erkennenden Subjekt auf der einen Seite und des erkannten Objektes auf der anderen Seite zu der Idee des Schnittes zwischen Beobachter oder Beobachtungsmittel und dem beobachteten System.’ (‘In this way, modern physics generalizes the old opposition between the knowing subject on the one hand and the known object on the other to the idea of the cut between observer or means of observation and the observed system.’) He then continued calling the cut a necessary condition for human knowledge: see footnote 72.

<sup>69</sup>Instead of ‘discreteness’, Bohr alternatively used the words ‘discontinuity’ or ‘individuality’

very existence of the quantum of action entails — because of the impossibility of controlling the reaction of the object on the measurement instruments if these are to serve their purpose — the necessity of a final renunciation of the classical ideal of causality and a radical revision of our attitude towards the problem of physical reality.’ Also, Heisenberg’s uncertainty relations were originally motivated by the quantum postulate in the above form. According to Bohr and Heisenberg around 1927, this ‘essential discreteness’ causes an ‘uncontrollable disturbance’ of the object by the apparatus during their interaction. Although the “quantum postulate” is not supported by the mature mathematical formalism of quantum mechanics and is basically obsolete, the intuition of Bohr and Heisenberg that a measurement of a quantum-mechanical object causes an ‘uncontrollable disturbance’ of the latter is actually quite right.<sup>70</sup>

In actual fact, the reason for this disturbance does not lie in the “quantum postulate”, but in the phenomenon of entanglement, as further discussed in Subsection 3.4. Namely, from the point of view of von Neumann’s measurement theory (see Subsection 2.5) the Heisenberg cut is just a two-step example of a von Neumann chain, with the special feature that after the quantum-mechanical interaction has taken place, the second link (i.e. the apparatus) is *described* classically. The latter feature not only supports Bohr’s philosophical agenda, but, more importantly, also suffices to guarantee the applicability of the ignorance interpretation of the mixed state that arises after completion of the measurement.<sup>71</sup> All of von Neumann’s analysis of the arbitrariness of the location of the cut applies here, for one may always extend the definition of the quantum-mechanical object by coupling the original choice to any other purely quantum-mechanical system one likes, and analogously for the classical part. Thus the two-step nature of the Heisenberg cut includes the possibility that the first link or object is in fact a lengthy chain in itself (as long as it is quantum-mechanical), and similarly for the second link (as long as it is classical).<sup>72</sup> This arbitrariness, subject to the limitation expressed by the second [1935] Bohr quote in this subsection, was well recognized by Bohr and Heisenberg, and was found at least by Bohr to be of great philosophical importance.

It is the interaction between object and apparatus that causes the measurement to ‘disturb’ the former, but it is only and precisely the classical description of

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as well. He rarely omitted amplifications like ‘essential’.

<sup>70</sup>Despite the fact that Bohr later distanced himself from it; cf. [Beller, 1999] and footnote 52 above. In a correct analysis, what is disturbed upon coupling to a classical apparatus is the quantum-mechanical state of the object (rather than certain sharp values of classical observables such as position and momentum, as the early writings of Bohr and Heisenberg suggest).

<sup>71</sup>In a purely quantum-mechanical von Neumann chain the final state of system plus apparatus is pure, but if the apparatus is classical, then the post-measurement state is mixed.

<sup>72</sup>Pauli [1949] once more: ‘Während die EXISTENZ eines solchen Schnittes eine notwendige Bedingung menschlicher Erkenntnis ist, faßt sie die LAGE des Schnittes als bis zu einem gewissen Grade willkürlich und als Resultat einer durch Zweckmäßigkeitserwägungen mitbestimmten, also teilweise freien Wahl auf.’ (‘While the EXISTENCE of such a [Heisenberg] cut is a necessary condition for human knowledge, its LOCATION is to some extent arbitrary as a result of a pragmatic and thereby partly free choice.’)

the latter that (through the ignorance interpretation of the final state) makes the disturbance ‘uncontrollable’.<sup>73</sup> In the Copenhagen interpretation, *probabilities arise solely because we look at the quantum world through classical glasses.*

‘Just the necessity of accounting for the function of the measuring agencies on classical lines excludes in principle in proper quantum phenomena an accurate control of the reaction of the measuring instruments on the atomic objects.’ [Bohr, 1956, 87]

‘One may call these uncertainties objective, in that they are simply a consequence of the fact that we describe the experiment in terms of classical physics; they do not depend in detail on the observer. One may call them subjective, in that they reflect our incomplete knowledge of the world.’ [Heisenberg, 1958, 53–54]

Thus the picture that arises is this: Although the quantum-mechanical side of the Heisenberg cut is described by the Schrödinger equation (which is deterministic), while the classical side is subject to Newton’s laws (which are equally well deterministic),<sup>74</sup> unpredictability arises because the quantum system serving as an apparatus is approximated by a classical system. The ensuing probabilities reflect the ignorance arising from the decision (or need) to ignore the quantum-mechanical degrees of freedom of the apparatus. Hence the probabilistic nature of quantum theory is not intrinsic but extrinsic, and as such is entirely a consequence of the doctrine of classical concepts, which by the same token *explains* this nature.

Mathematically, the simplest illustration of this idea is as follows. Take a finite-dimensional Hilbert space  $\mathcal{H} = \mathbb{C}^n$  with the ensuing algebra of observables  $\mathcal{A} = M_n(\mathbb{C})$  (i.e. the  $n \times n$  matrices). A unit vector  $\Psi \in \mathbb{C}^n$  determines a quantum-mechanical state in the usual way. Now describe this quantum system as if it were classical by ignoring all observables except the diagonal matrices. The state then immediately collapses to a probability measure on the set of  $n$  points, with probabilities given by the Born rule  $p(i) = |(e_i, \Psi)|^2$ , where  $(e_i)_{i=1, \dots, n}$  is the standard basis of  $\mathbb{C}^n$ . Similarly, the Born–Pauli rule for the probabilistic interpretation of the wave function  $\Psi \in L^2(\mathbb{R}^3)$  in terms of  $|\Psi(x)|^2$  immediately follows if one ignores all observables on  $L^2(\mathbb{R}^3)$  except the position operator.<sup>75</sup>

Despite the appeal of this entire picture, it is not at all clear that it actually applies! There is no a priori guarantee whatsoever that one may indeed describe a quantum system “as if it were classical”. Bohr and Heisenberg apparently took the existence of the classical world of mountains and creeks they loved so much for granted, the former probably on empirical grounds, the latter on the basis of his

<sup>73</sup>These points were not clearly separated by Heisenberg [1927] in his paper on the uncertainty relations, but were later clarified by Bohr. See [Scheibe, 1973].

<sup>74</sup>But see [Earman, 1986; 2005].

<sup>75</sup>Technically, one restricts  $\Psi$  — seen as a state on the  $C^*$ -algebra  $\mathcal{B}(L^2(\mathbb{R}^3))$  — to the  $C^*$ -algebra  $C_0(\mathbb{R}^3)$  given by all multiplication operators on  $L^2(\mathbb{R}^3)$  defined by continuous functions of  $x \in \mathbb{R}^3$  that vanish at infinity. This restriction yields a probability measure on  $\mathbb{R}^3$ , which is precisely the usual one originally proposed by Pauli.



own uncertainty relations — both almost blind to the extremely delicate mathematical and conceptual problems involved. In our opinion, the main difficulty in making sense of the Copenhagen interpretation therefore lies in the justification of the classical description in question. This difficulty is the main topic of this paper, of which Section 6 is of particular relevance in the present context.

### 3.3 Complementarity

The notion of a Heisenberg cut is subject to a certain arbitrariness even apart from the precise location of the cut within a given chain, for one might in principle construct the chain in various different and incompatible ways. This arbitrariness was analyzed by Bohr in terms of what he called *complementarity*.<sup>76</sup>

Bohr never gave a precise definition of complementarity,<sup>77</sup> but restricted himself to the analysis of a number of examples.<sup>78</sup> A prominent such example is the complementarity between a “causal”<sup>79</sup> description of a quantum system in which conservation laws hold, and a space-time description that is necessarily statistical in character. Here Bohr’s idea seems to have been that a stationary state (i.e. an energy eigenstate) of an atom is incompatible with an electron moving in its orbit in space and time — see Subsection 5.4 for a discussion of this issue. Heisenberg [1958], however, took this example of complementarity to mean that a system on which no measurement is performed evolves deterministically according to the Schrödinger equation, whereas a rapid succession of measurements produces a space-time path whose precise form quantum theory is only able to predict statistically [Camilleri, 2005]. In other words, this example reproduces precisely the picture through which Heisenberg [1927] believed he had established the connection between classical and quantum mechanics; cf. Subsection 2.3.

Bohr’s other key example was the complementarity between particles and waves. Here his principal aim was to make sense of Young’s double-slit experiment. The well-known difficulty with a classical visualization of this experiment is that a particle description appears impossible because a particle has to go through a single slit, ruining the interference pattern gradually built up on the detection screen, whereas a wave description seems incompatible with the point-like localization on the screen once the wave hits it. Thus Bohr suggested that whilst each of these classical descriptions is incomplete, the union of them is necessary for a complete

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<sup>76</sup>Unfortunately and typically, Bohr once again presented complementarity as a necessity of thought rather than as the truly amazing possible mode of description it really is.

<sup>77</sup>Perhaps he preferred this approach because he felt a definition could only reveal part of what was supposed to be defined: one of his favourite examples of complementarity was that between definition and observation.

<sup>78</sup>We refrain from discussing the complementarity between truth and clarity, science and religion, thoughts and feelings, and objectivity and introspection here, despite the fact that on this basis Bohr’s biographer Pais [1997] came to regard his subject as the greatest philosopher since Kant.

<sup>79</sup>Bohr’s use the word “causal” is quite confusing in view of the fact that in the British empiricist tradition causality is often interpreted in the sense of a space-time description. But Bohr’s “causal” is meant to be *complementary* to a space-time description!

description of the experiment.

The deeper epistemological point appears to be that although the *completeness* of the quantum-mechanical description of the microworld systems seems to be endangered by the doctrine of classical concepts, it is actually restored by the inclusion of *two* “complementary” descriptions (i.e. of a given quantum system plus a measuring device that is necessarily described classically, ‘if it is to serve its purpose’). Unfortunately, despite this attractive general idea it is unclear to what precise definition of complementarity Bohr’s examples should lead. In the first, the complementary notions of determinism and a space-time description are in mutual harmony as far as classical physics is concerned, but are apparently in conflict with each other in quantum mechanics. In the second, however, the wave description of some entity contradicts a particle description of the same entity precisely in classical physics, whereas in quantum mechanics these descriptions somehow coexist.<sup>80</sup>

Scheibe [1973, 32] notes a ‘clear convergence [in the writings of Bohr] towards a preferred expression of a complementarity between phenomena’, where a Bohrian *phenomenon* is an indivisible union (or “whole”) of a quantum system and a classically described experimental arrangement used to study it; see item 2 below. Some of Bohr’s early examples of complementarity can be brought under this heading, others cannot [Held, 1994]. For many students of Bohr (including the present author), the fog has yet to clear up.<sup>81</sup> Nonetheless, the following mathematical interpretations might assign some meaning to the idea of complementarity in the framework of von Neumann’s formalism of quantum mechanics.<sup>82</sup>

1. Heisenberg [1958] *identified complementary pictures of a quantum-mechanical system with equivalent mathematical representations thereof*. For example, he thought of the complementarity of  $x$  and  $p$  as the existence of what we now call the Schrödinger representations of the canonical commutation relations (CCR) on  $L^2(\mathbb{R}^n)$  and its Fourier transform to momentum space. Furthermore, he felt that in quantum field theory particles and waves gave two *equivalent* modes of description of quantum theory because of second quantization. Thus for Heisenberg complementary pictures are classical because there is an underlying classical variable, with no apparatus in sight, and such pictures are not mutually contradictory but (unitarily) equivalent.

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<sup>80</sup>On top of this, Bohr mixed these examples in conflicting ways. In discussing bound states of electrons in an atom he jointly made determinism and particles one half of a complementary pair, waves and space-time being the other. In his description of electron-photon scattering he did it the other way round: this time determinism and waves formed one side, particles and space-time the other (cf. [Beller, 1999]).

<sup>81</sup>Even Einstein [1949, 674] conceded that throughout his debate with Bohr he had never understood the notion of complementarity, ‘the sharp formulation of which, moreover, I have been unable to achieve despite much effort which I have expended on it.’ See [Landsman, 2006b] for the author’s view on the Bohr–Einstein debate.

<sup>82</sup>This exercise is quite against the spirit of Bohr, who is on record as saying that ‘von Neumann’s approach (...) did not *solve* problems but created *imaginary difficulties* ([Scheibe, 1973, 11], quoting Feyerabend; italics in original).

See also [Camilleri, 2005, 88], according to whom ‘Heisenberg never accepted Bohr’s complementarity arguments’.

2. Pauli [1933] simply stated that *two observables are complementary when the corresponding operators fail to commute*.<sup>83</sup> Consequently, it then follows from Heisenberg’s uncertainty relations that complementary observables cannot be measured simultaneously with arbitrary precision. This suggests (but by no means proves) that they should be measured independently, using mutually exclusive experimental arrangements. The latter feature of complementarity was emphasized by Bohr in his later writings.<sup>84</sup> This approach makes the notion of complementarity unambiguous and mathematically precise, and perhaps for this reason the few physicists who actually use the idea of complementarity in their work tend to follow Pauli and the later Bohr.<sup>85</sup>
3. The present author proposes that *observables and pure states are complementary*. For in the Schrödinger representation of elementary quantum mechanics, the former are, roughly speaking, generated by the position and

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<sup>83</sup>More precisely, one should probably require that the two operators in question generate the ambient algebra of observables, so that complementarity in Pauli’s sense is really defined between two commutative subalgebras of a given algebra of observables (again, provided they jointly generate the latter).

<sup>84</sup>Bohr’s earlier writings do not quite conform to Pauli’s approach [Scheibe, 1973; Held, 1994]. In Bohr’s discussions of the double-slit experiment particle and wave form a complementary pair, whereas Pauli’s complementary observables are position and momentum, which refer to a single side of Bohr’s pair. For a precise analysis of the relationship between mutually exclusive experimental arrangements, non-commuting observables, and the Heisenberg uncertainty relations see [Busch *et al.*, 1998] and [De Muynck, 2002].

<sup>85</sup>Adopting this point of view, it is tempting to capture the complementarity between position and momentum by means of the following conjecture: *Any normal pure state  $\omega$  on  $\mathcal{B}(L^2(\mathbb{R}^n))$  (that is, any wave function seen as a state in the sense of  $C^*$ -algebras) is determined by the pair  $\{\omega|L^\infty(\mathbb{R}^n), \omega|FL^\infty(\mathbb{R}^n)F^{-1}\}$  (in other words, by its restrictions to position and momentum). Here  $L^\infty(\mathbb{R}^n)$  is the von Neumann algebra of multiplication operators on  $L^2(\mathbb{R}^n)$ , i.e. the von Neumann algebra generated by the position operator, whereas  $FL^\infty(\mathbb{R}^n)F^{-1}$  is its Fourier transform, i.e. the von Neumann algebra generated by the momentum operator. The idea is that each of its restrictions  $\omega|L^\infty(\mathbb{R}^n)$  and  $\omega|FL^\infty(\mathbb{R}^n)F^{-1}$  gives a classical picture of  $\omega$ . These restrictions are a measure on  $\mathbb{R}^n$  interpreted as position space, and another measure on  $\mathbb{R}^n$  interpreted as momentum space. Unfortunately, this conjecture is false. The following counterexample was provided by D. Buchholz (private communication): take  $\omega$  as the state defined by the wave function  $\Psi(x) \sim \exp(-ax^2/2)$  with  $\text{Re}(a) > 0$ ,  $\text{Im}(a) \neq 0$ , and  $|a|^2 = 1$ . Then  $\omega$  depends on  $\text{Im}(a)$ , whereas neither  $\omega|L^\infty(\mathbb{R}^n)$  nor  $\omega|FL^\infty(\mathbb{R}^n)F^{-1}$  does. There is even a counterexample to the analogous conjecture for the  $C^*$ -algebra of  $2 \times 2$  matrices, found by H. Halvorson: if  $A$  is the commutative  $C^*$ -algebra generated by  $\sigma_x$ , and  $B$  the one generated by  $\sigma_y$ , then the two different eigenstates of  $\sigma_z$  coincide on  $A$  and on  $B$ . One way to improve our conjecture might be to hope that if, in the Schrödinger picture, two states coincide on the two given commutative von Neumann algebras for all times, then they must be equal. But this can only be true for certain “realistic” time-evolutions, for the trivial Hamiltonian  $H = 0$  yields the above counterexample. We leave this as a problem for future research. At the time of writing, Halvorson [2004] contains the only sound mathematical interpretation of the complementarity between position and momentum, by relating it to the representation theory of the CCR. He shows that in any representation where the position operator has eigenstates, there is no momentum operator, and vice versa.*

momentum operators, whereas the latter are given by wave functions. Some of Bohr's other examples of complementarity also square with this interpretation (at least if one overlooks the collapse of the wavefunction upon a measurement). Here one captures the idea that both ingredients of a complementary pair are necessary for a complete description, though the alleged mutual contradiction between observables and states is vague. Also, this reading of complementarity relies on a specific representation of the canonical commutation relations. It is not quite clear what one gains with this ideology, but perhaps it deserves to be developed in some more detail. For example, in quantum field theory it is once more the observables that carry the space-time description, especially in the algebraic description of Haag [1992].

### 3.4 *Epilogue: entanglement to the rescue?*

Bohr's "quantum postulate" being obscure and obsolete, it is interesting to consider Howard's [1994] 'reconstruction' of Bohr's philosophy of physics on the basis of entanglement.<sup>86</sup> His case can perhaps be strengthened by an appeal to the analysis Primas [1983] has given of the need for classical concepts in quantum physics.<sup>87</sup> Primas proposes to define a "quantum object" as a physical system  $S$  that is free from what he calls "EPR-correlations" with its environment. Here the "environment" is meant to include apparatus, observer, the rest of the universe if necessary, and what not. In elementary quantum mechanics, quantum objects in this sense exist only in very special states: if  $\mathcal{H}_S$  is the Hilbert space of the system  $S$ , and  $\mathcal{H}_E$  that of the environment  $E$ , any pure state of the form  $\sum_i c_i \Psi_i \otimes \Phi_i$  (with more than one term) by definition correlates  $S$  with  $E$ ; the only uncorrelated pure states are those of the form  $\Psi \otimes \Phi$  for unit vectors  $\Psi \in \mathcal{H}_S$ ,  $\Phi \in \mathcal{H}_E$ . The restriction of a pure EPR-correlated state on  $S + E$  to  $S$  is mixed, so that the (would-be) quantum object 'does not have its own pure state'; in other words, the restriction of an EPR-correlated state  $\omega$  to  $S$  together with its restriction to  $E$  do not jointly determine  $\omega$ . More generally, if the state of  $S + E$  is EPR-correlated, a complete characterization of the state of  $S$  requires  $E$  (and vice versa). But (against Bohr!) mathematics defeats words: the sharpest characterization of the notion of EPR-correlations can be given in terms of operator algebras, as follows. In the spirit of the remainder of the paper we proceed in a rather general and abstract way.<sup>88</sup> For what follows see especially [Werner, 1989].

<sup>86</sup>We find little evidence that Bohr himself ever thought along those lines. With approval we quote Zeh, who, following a statement of the quantum postulate by Bohr similar to the one in Subsection 3.2 above, writes: 'The later revision of these early interpretations of quantum theory (required by the important role of entangled quantum states for much larger systems) seems to have gone unnoticed by many physicists.' [Joos *et al.*, 2003, 23] See also [Howard, 1990] for an interesting historical perspective on entanglement, and cf. [Raimond *et al.*, 2001] for the experimental situation.

<sup>87</sup>See also [Amann and Primas, 1997] and [Primas, 1997].

<sup>88</sup>Summers and Werner [1987] give even more general results, where the tensor product  $\mathcal{A} \hat{\otimes} \mathcal{B}$  below is replaced by an arbitrary  $C^*$ -algebra  $\mathcal{C}$  containing  $\mathcal{A}$  and  $\mathcal{B}$  as  $C^*$ -subalgebras.

Let  $\mathcal{A}$  and  $\mathcal{B}$  be  $C^*$ -algebras,<sup>89</sup> with tensor product  $\mathcal{A} \hat{\otimes} \mathcal{B}$ .<sup>90</sup> Less abstractly, just think of two Hilbert spaces  $\mathcal{H}_S$  and  $\mathcal{H}_E$  as above, with tensor product  $\mathcal{H}_S \otimes \mathcal{H}_E$ , and assume that  $\mathcal{A} = \mathcal{B}(\mathcal{H}_S)$  while  $\mathcal{B}$  is either  $\mathcal{B}(\mathcal{H}_E)$  itself or some (norm-closed and involutive) commutative subalgebra thereof. The tensor product  $\mathcal{A} \hat{\otimes} \mathcal{B}$  is then a (norm-closed and involutive) subalgebra of  $\mathcal{B}(\mathcal{H}_S \otimes \mathcal{H}_E)$ , the algebra of all bounded operators on  $\mathcal{H}_S \otimes \mathcal{H}_E$ .

A *product state* on  $\mathcal{A} \hat{\otimes} \mathcal{B}$  is a state of the form  $\omega = \rho \otimes \sigma$ , where the states  $\rho$  on  $\mathcal{A}$  and  $\sigma$  on  $\mathcal{B}$  may be either pure or mixed.<sup>91</sup> We say that a state  $\omega$  on  $\mathcal{A} \hat{\otimes} \mathcal{B}$  is *decomposable* when it is a mixture of product states, i.e. when  $\omega = \sum_i p_i \rho_i \otimes \sigma_i$ , where the coefficients  $p_i > 0$  satisfy  $\sum_i p_i = 1$ .<sup>92</sup> A decomposable state  $\omega$  is pure precisely when it is a product of pure states. This has the important consequence that both its restrictions  $\omega|_{\mathcal{A}}$  and  $\omega|_{\mathcal{B}}$  to  $\mathcal{A}$  and  $\mathcal{B}$ , respectively, are pure as well.<sup>93</sup> On the other hand, a state on  $\mathcal{A} \hat{\otimes} \mathcal{B}$  may be said to be *EPR-correlated* [Primas, 1983] when it is *not* decomposable. An EPR-correlated *pure* state has the property that its restriction to  $\mathcal{A}$  or  $\mathcal{B}$  is *mixed*.

Raggio [1981] proved that the following two conditions are equivalent:

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<sup>89</sup> Recall that a  $C^*$ -algebra is a complex algebra  $\mathcal{A}$  that is complete in a norm  $\|\cdot\|$  that satisfies  $\|AB\| \leq \|A\| \|B\|$  for all  $A, B \in \mathcal{A}$ , and has an involution  $A \rightarrow A^*$  such that  $\|A^*A\| = \|A\|^2$ . A basic example is  $\mathcal{A} = \mathcal{B}(\mathcal{H})$ , the algebra of all bounded operators on a Hilbert space  $\mathcal{H}$ , equipped with the usual operator norm and adjoint. By the Gelfand–Naimark theorem, any  $C^*$ -algebra is isomorphic to a norm-closed self-adjoint subalgebra of  $\mathcal{B}(\mathcal{H})$ , for some Hilbert space  $\mathcal{H}$ . Another key example is  $\mathcal{A} = C_0(X)$ , the space of all continuous complex-valued functions on a (locally compact Hausdorff) space  $X$  that vanish at infinity (in the sense that for every  $\varepsilon > 0$  there is a *compact* subset  $K \subset X$  such that  $|f(x)| < \varepsilon$  for all  $x \notin K$ ), equipped with the supremum norm  $\|f\|_\infty := \sup_{x \in X} |f(x)|$ , and involution given by (pointwise) complex conjugation. By the Gelfand–Naimark lemma, any commutative  $C^*$ -algebra is isomorphic to  $C_0(X)$  for some locally compact Hausdorff space  $X$ .

<sup>90</sup> The tensor product of two (or more)  $C^*$ -algebras is not unique, and we here need the so-called *projective* tensor product  $\mathcal{A} \hat{\otimes} \mathcal{B}$ , defined as the completion of the algebraic tensor product  $\mathcal{A} \otimes \mathcal{B}$  in the *maximal*  $C^*$ -cross-norm. The choice of the projective tensor product guarantees that each state on  $\mathcal{A} \otimes \mathcal{B}$  extends to a state on  $\mathcal{A} \hat{\otimes} \mathcal{B}$  by continuity; conversely, since  $\mathcal{A} \otimes \mathcal{B}$  is dense in  $\mathcal{A} \hat{\otimes} \mathcal{B}$ , each state on the latter is uniquely determined by its values on the former. See [Wegge-Olsen, 1993, Appendix T], or [Takesaki, 2003, Vol. I, Ch. IV]. In particular, product states  $\rho \otimes \sigma$  and mixtures  $\omega = \sum_i p_i \rho_i \otimes \sigma_i$  thereof as considered below are well defined on  $\mathcal{A} \hat{\otimes} \mathcal{B}$ . If  $\mathcal{A} \subset \mathcal{B}(\mathcal{H}_S)$  and  $\mathcal{B} \subset \mathcal{B}(\mathcal{H}_E)$  are von Neumann algebras, as in the analysis of Raggio [1981; 1988], it is easier (and sufficient) to work with the *spatial* tensor product  $\mathcal{A} \overline{\otimes} \mathcal{B}$ , defined as the double commutant (or weak completion) of  $\mathcal{A} \otimes \mathcal{B}$  in  $\mathcal{B}(\mathcal{H}_S \otimes \mathcal{H}_E)$ . For any *normal* state on  $\mathcal{A} \otimes \mathcal{B}$  extends to a normal state on  $\mathcal{A} \overline{\otimes} \mathcal{B}$  by continuity.

<sup>91</sup> We use the notion of a state that is usual in the algebraic framework. Hence a *state* on a  $C^*$ -algebra  $\mathcal{A}$  is a linear functional  $\rho : \mathcal{A} \rightarrow \mathbb{C}$  that is *positive* in that  $\rho(A^*A) \geq 0$  for all  $A \in \mathcal{A}$  and *normalized* in that  $\rho(1) = 1$ , where 1 is the unit element of  $\mathcal{A}$ . If  $\mathcal{A}$  is a von Neumann algebra, one has the notion of a *normal* state, which satisfies an additional continuity condition. If  $\mathcal{A} = \mathcal{B}(\mathcal{H})$ , then a fundamental theorem of von Neumann states that each normal state  $\rho$  on  $\mathcal{A}$  is given by a density matrix  $\hat{\rho}$  on  $\mathcal{H}$ , so that  $\rho(A) = \text{Tr}(\hat{\rho}A)$  for each  $A \in \mathcal{A}$ . In particular, a normal pure state on  $\mathcal{B}(\mathcal{H})$  (seen as a von Neumann algebra) is necessarily of the form  $\psi(A) = (\Psi, A\Psi)$  for some unit vector  $\Psi \in \mathcal{H}$ .

<sup>92</sup> Infinite sums are allowed here. More precisely,  $\omega$  is decomposable if it is in the  $w^*$ -closure of the convex hull of the product states on  $\mathcal{A} \hat{\otimes} \mathcal{B}$ .

<sup>93</sup> The restriction  $\omega|_{\mathcal{A}}$  of a state  $\omega$  on  $\mathcal{A} \hat{\otimes} \mathcal{B}$  to, say,  $\mathcal{A}$  is given by  $\omega|_{\mathcal{A}}(A) = \omega(A \otimes 1)$ , where 1 is the unit element of  $\mathcal{B}$ , etc.

- Each state on  $\mathcal{A} \hat{\otimes} \mathcal{B}$  is decomposable;
- $\mathcal{A}$  or  $\mathcal{B}$  is commutative.

In other words, EPR-correlated states exist precisely when  $\mathcal{A}$  and  $\mathcal{B}$  are both non-commutative.<sup>94</sup> As one might expect, this result is closely related to the Bell inequalities. Namely, consider the inequality

$$(1) \quad |\sup\{\omega(A_1(B_1 + B_2) + A_2(B_1 - B_2))\}| \leq 2,$$

where  $\omega$  is a fixed state on  $\mathcal{A} \hat{\otimes} \mathcal{B}$  and the supremum is taken over all self-adjoint operators  $A_1, A_2 \in \mathcal{A}$ ,  $B_1, B_2 \in \mathcal{B}$ , each of norm  $\leq 1$ . Eq. (1) holds if and only if  $\omega$  is decomposable [Baez, 1987; Raggio, 1988]. Consequently, the inequality (1) can only be violated in some state  $\omega$  when the algebras  $\mathcal{A}$  and  $\mathcal{B}$  are both noncommutative. If, on the other hand, (1) is satisfied, then one knows that there exists a classical probability space and probability measure (and hence a “hidden variables” theory) reproducing the given correlations [Pitowsky, 1989]. As stressed by Bacciagaluppi [1993], such a description does *not* require the entire setting to be classical; as we have seen, only one of the algebras  $\mathcal{A}$  and  $\mathcal{B}$  has to be commutative for the Bell inequalities to hold.

Where does this leave us with respect to Bohr? If we follow Primas [1983] in describing a (quantum) object as a system free from EPR-correlations with its environment, then the mathematical results just reviewed leave us with two possibilities. Firstly, we may pay lip-service to Bohr in taking the algebra  $\mathcal{B}$  (interpreted as the algebra of observables of the environment in the widest possible sense, as above) to be commutative *as a matter of description*. In that case, our object is really an “object” in *any* of its states. But clearly this is not the only possibility. For even in the case of elementary quantum mechanics — where  $\mathcal{A} = \mathcal{B}(\mathcal{H}_S)$  and  $\mathcal{B} = \mathcal{B}(\mathcal{H}_E)$  — the system is still an “object” in the sense of Primas as long as the total state  $\omega$  of  $S + E$  is decomposable. In general, for pure states this just means that  $\omega = \psi \otimes \phi$ , i.e. that the total state is a product of pure states. To accomplish this, one has to define the Heisenberg cut in an appropriate way, and subsequently hope that the given product state remains so under time-evolution (see [Amann and Primas, 1997] and [Atmanspacher *et al.*, 1999], and references therein). This selects certain states on  $\mathcal{A}$  as “robust” or “stable”, in much the same way as in the decoherence approach. We therefore continue this discussion in Section 7 (see especially point 6 in Subsection 7.1).

## 4 QUANTIZATION

Heisenberg’s [1925] idea of *Umdeutung* (*reinterpretation*) suggests that it is possible to construct a quantum-mechanical description of a physical system whose classical description is known. As we have seen, this possibility was realized by Schrödinger

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<sup>94</sup>Raggio [1981] proved this for von Neumann algebras and normal states. His proof was adapted to  $C^*$ -algebras by Bacciagaluppi [1993].

[1925c], who found the simplest example (2) and (3) of *Umdeutung* in the context of atomic physics. This early example was phenomenally successful, as almost all of atomic and molecular physics is still based on it.

Quantization theory is an attempt to understand this example, make it mathematically precise, and generalize it to more complicated systems. It has to be stated from the outset that, like the entire classical-quantum interface, the nature of quantization is not yet well understood. This fact is reflected by the existence of a fair number of competing quantization procedures, the most transparent of which we will review below.<sup>95</sup> Among the first mathematically serious discussions of quantization are [Mackey, 1968] and [Souriau, 1969]; more recent and comprehensive treatments are, for example, [Woodhouse, 1992; Landsman, 1998], and [Ali and Englis, 2004].

#### 4.1 Canonical quantization and systems of imprimitivity

The approach based on (2) is often called *canonical quantization*. Even apart from the issue of mathematical rigour, one can only side with Mackey [1992, 283], who wrote: ‘Simple and elegant as this model is, it appears at first sight to be quite arbitrary and ad hoc. It is difficult to understand how anyone could have guessed it and by no means obvious how to modify it to fit a model for space different from  $\mathbb{R}^r$ .’

One veil of the mystery of quantization was lifted by von Neumann [1931], who (following earlier heuristic proposals by Heisenberg, Schrödinger, Dirac, and Pauli) recognized that (2) does not merely provide a representation of the canonical commutation relations

$$(1) \quad [\mathcal{Q}_{\hbar}(p_j), \mathcal{Q}_{\hbar}(q^k)] = -i\hbar\delta_j^k,$$

but (subject to a regularity condition)<sup>96</sup> is *the only* such representation that is irreducible (up to unitary equivalence). In particular, the seemingly different formulations of quantum theory by Heisenberg and Schrödinger (amended by the inclusion of states and of observables, respectively — cf. Section 2) simply involved superficially different but unitarily equivalent representations of (1): the difference between matrices and waves was just one between coordinate systems in Hilbert space, so to speak. Moreover, any other conceivable formulation of quan-

<sup>95</sup>The path integral approach to quantization is still under development and so far has had no impact on foundational debates, so we will not discuss it here. See [Albeverio and Høegh-Krohn, 1976] and [Glimm and Jaffe, 1987].

<sup>96</sup>It is required that the unbounded operators  $\mathcal{Q}_{\hbar}(p_j)$  and  $\mathcal{Q}_{\hbar}(q^k)$  integrate to a unitary representation of the  $2n + 1$ -dimensional Heisenberg group  $H_n$ , i.e. the unique connected and simply connected Lie group with  $2n + 1$ -dimensional Lie algebra with generators  $X_i, Y_i, Z$  ( $i = 1, \dots, n$ ) subject to the Lie brackets  $[X_i, X_j] = [Y_i, Y_j] = 0$ ,  $[X_i, Y_j] = \delta_{ij}Z$ ,  $[X_i, Z] = [Y_i, Z] = 0$ . Thus von Neumann’s uniqueness theorem for representations of the canonical commutation relations is (as he indeed recognized himself) really a uniqueness theorem for unitary representations of  $H_n$  for which the central element  $Z$  is mapped to  $-i\hbar^{-1}1$ , where  $\hbar \neq 0$  is a *fixed* constant. See, for example, [Corwin and Greenleaf, 1989] or [Landsman, 1998].

tum mechanics — now simply *defined* as a (regular) Hilbert space representation of (1) — has to be equivalent to the one of Heisenberg and Schrödinger.<sup>97</sup>

This, then, transfers the quantization problem of a particle moving on  $\mathbb{R}^n$  to the canonical commutation relations (1). Although a mathematically rigorous theory of these commutation relations (as they stand) exists [Jørgensen and Moore, 1984; Schmüdgen, 1990], they are problematic nonetheless. Firstly, technically speaking the operators involved are unbounded, and in order to represent physical observables they have to be self-adjoint; yet on their respective domains of self-adjointness the commutator on the left-hand side is undefined. Secondly, and more importantly, (1) relies on the possibility of choosing global coordinates on  $\mathbb{R}^n$ , which precludes a naive generalization to arbitrary configuration spaces. And thirdly, even if one has managed to quantize  $p$  and  $q$  by finding a representation of (1), the problem of quantizing other observables remains — think of the Hamiltonian and the Schrödinger equation.

About 50 years ago, Mackey set himself the task of making good sense of canonical quantization; see [Mackey, 1968; 1978; 1992] and the brief exposition below for the result. Although the author now regards Mackey's reformulation of quantization in terms of induced representations and systems of imprimitivity merely as a stepping stone towards our current understanding based on deformation theory and groupoids (cf. Subsection 4.3 below), Mackey's approach is (quite rightly) often used in the foundations of physics, and one is well advised to be familiar with it. In any case, Mackey [1992, 283] — continuing the previous quotation) claims with some justification that his approach to quantization 'removes much of the mystery.'

Like most approaches to quantization, Mackey assigns momentum and position a quite different role in quantum mechanics, despite the fact that in classical mechanics  $p$  and  $q$  can be interchanged by a canonical transformation.<sup>98</sup>

1. The position operators  $Q_{\hbar}(q^j)$  are collectively replaced by a single projection-valued measure  $P$  on  $\mathbb{R}^n$ ,<sup>99</sup> which on  $L^2(\mathbb{R}^n)$  is given by  $P(E) = \chi_E$  as a multiplication operator. Given this  $P$ , any multiplication operator defined by a (measurable) function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  can be represented as  $\int_{\mathbb{R}^n} dP(x) f(x)$ , which is defined and self-adjoint on a suitable domain.<sup>100</sup> In particular, the position operators  $Q_{\hbar}(q^j)$  can be reconstructed from  $P$  by choosing  $f(x) =$

<sup>97</sup>This is unrelated to the issue of the Heisenberg picture versus the Schrödinger picture, which is about the time-evolution of observables versus that of states.

<sup>98</sup>Up to a minus sign, that is. This is true globally on  $\mathbb{R}^n$  and locally on any symplectic manifold, where local Darboux coordinates do not distinguish between position and momentum.

<sup>99</sup>A projection-valued measure  $P$  on a space  $\Omega$  with Borel structure (i.e. equipped with a  $\sigma$ -algebra of measurable sets defined by the topology) with values in a Hilbert space  $\mathcal{H}$  is a map  $E \mapsto P(E)$  from the Borel subsets  $E \subset \Omega$  to the projections on  $\mathcal{H}$  that satisfies  $P(\emptyset) = 0$ ,  $P(\Omega) = 1$ ,  $P(E)P(F) = P(F)P(E) = P(E \cap F)$  for all measurable  $E, F \subset \Omega$ , and  $P(\cup_{i=1}^{\infty} E_i) = \sum_{i=1}^{\infty} P(E_i)$  for all countable collections of mutually disjoint  $E_i \subset \Omega$ .

<sup>100</sup>This domain consists of all  $\Psi \in \mathcal{H}$  for which  $\int_{\mathbb{R}^n} d(\Psi, P(x)\Psi) |f(x)|^2 < \infty$ .



$x^j$ , i.e.

$$(2) \quad \mathcal{Q}_\hbar(q^j) = \int_{\mathbb{R}^n} dP(x) x^j.$$

2. The momentum operators  $\mathcal{Q}_\hbar(p_j)$  are collectively replaced by a single unitary group representation  $U(\mathbb{R}^n)$ , defined on  $L^2(\mathbb{R}^n)$  by

$$U(y)\Psi(x) := \Psi(x - y).$$

Each  $\mathcal{Q}_\hbar(p_j)$  can be reconstructed from  $U$  by means of

$$(3) \quad \mathcal{Q}_\hbar(p_j)\Psi := i\hbar \lim_{t_j \rightarrow 0} t_j^{-1}(U(t_j) - 1)\Psi,$$

where  $U(t_j)$  is  $U$  at  $x^j = t_j$  and  $x^k = 0$  for  $k \neq j$ .<sup>101</sup>

Consequently, it entails no loss of generality to work with the pair  $(P, U)$  instead of the pair  $(\mathcal{Q}_\hbar(q^k), \mathcal{Q}_\hbar(p_j))$ . The commutation relations (1) are now replaced by

$$(4) \quad U(x)P(E)U(x)^{-1} = P(xE),$$

where  $E$  is a (Borel) subset of  $\mathbb{R}^n$  and  $xE = \{x\omega \mid \omega \in E\}$ . On the basis of this reformulation, Mackey proposed the following sweeping generalization of the the canonical commutation relations:<sup>102</sup>

A *system of imprimitivity*  $(\mathcal{H}, U, P)$  for a given action of a group  $G$  on a space  $Q$  consists of a Hilbert space  $\mathcal{H}$ , a unitary representation  $U$  of  $G$  on  $\mathcal{H}$ , and a projection-valued measure  $E \mapsto P(E)$  on  $Q$  with values in  $\mathcal{H}$ , such that (4) holds for all  $x \in G$  and all Borel sets  $E \subset Q$ .

In physics such a system describes the quantum mechanics of a particle moving on a configuration space  $Q$  on which  $G$  acts by symmetry transformations; see Subsection 4.3 for a more detailed discussion. When everything is smooth,<sup>103</sup> each element  $X$  of the Lie algebra  $\mathfrak{g}$  of  $G$  defines a generalized momentum operator

$$(5) \quad \mathcal{Q}_\hbar(X) = i\hbar dU(X)$$

on  $\mathcal{H}$ .<sup>104</sup> These operators satisfy the generalized canonical commutation relations<sup>105</sup>

$$(6) \quad [\mathcal{Q}_\hbar(X), \mathcal{Q}_\hbar(Y)] = i\hbar \mathcal{Q}_\hbar([X, Y]).$$

<sup>101</sup>By Stone's theorem (cf. Reed and Simon, 1972), this operator is defined and self-adjoint on the set of all  $\Psi \in H$  for which the limit exists.

<sup>102</sup>All groups and spaces are supposed to be locally compact, and actions and representations are assumed continuous.

<sup>103</sup>I.e.  $G$  is a Lie group,  $Q$  is a manifold, and the  $G$ -action is smooth.

<sup>104</sup>This operator is defined and self-adjoint on the domain of vectors  $\Psi \in \mathcal{H}$  for which  $dU(X)\Psi := \lim_{t \rightarrow 0} t^{-1}(U(\exp(tX)) - 1)\Psi$  exists.

<sup>105</sup>As noted before in the context of (1), the commutation relations (6), (8) and (9) do not hold on the domain of self-adjointness of the operators involved, but on a smaller common core.

Furthermore, in terms of the operators<sup>106</sup>

$$(7) \quad \mathcal{Q}_\hbar(f) = \int_Q dP(x) f(x),$$

where  $f$  is a smooth function on  $Q$  and  $X \in \mathfrak{g}$ , one in addition has

$$(8) \quad [\mathcal{Q}_\hbar(X), \mathcal{Q}_\hbar(f)] = i\hbar \mathcal{Q}_\hbar(\xi_X^Q f),$$

where  $\xi_X^Q$  is the canonical vector field on  $Q$  defined by the  $G$ -action,<sup>107</sup> and

$$(9) \quad [\mathcal{Q}_\hbar(f_1), \mathcal{Q}_\hbar(f_2)] = 0.$$

Elementary quantum mechanics on  $\mathbb{R}^n$  corresponds to the special case  $Q = \mathbb{R}^n$  and  $G = \mathbb{R}^n$  with the usual additive group structure. To see this, we denote the standard basis of  $\mathbb{R}^3$  (in its guise as the Lie algebra of  $\mathbb{R}^3$ ) by the name  $(p_j)$ , and furthermore take  $f_1(q) = q^j$ ,  $f_2(q) = f(q) = q^k$ . Eq. (6) for  $X = p_j$  and  $Y = p_k$  then reads  $[\mathcal{Q}_\hbar(p_j), \mathcal{Q}_\hbar(p_k)] = 0$ , eq. (8) yields the canonical commutation relations (1), and (9) states the commutativity of the position operators, i.e.  $[\mathcal{Q}_\hbar(q^j), \mathcal{Q}_\hbar(q^k)] = 0$ .

In order to incorporate spin, one picks  $G = E(3) = SO(3) \times \mathbb{R}^3$  (i.e. the Euclidean motion group), acting on  $Q = \mathbb{R}^3$  in the obvious (defining) way. The Lie algebra of  $E(3)$  is  $\mathbb{R}^6 = \mathbb{R}^3 \times \mathbb{R}^3$  as a vector space; we extend the basis  $(p_j)$  of the second copy of  $\mathbb{R}^3$  (i.e. the Lie algebra of  $\mathbb{R}^3$ ) by a basis  $(J_i)$  of the first copy of  $\mathbb{R}^3$  (in its guise as the Lie algebra of  $SO(3)$ ), and find that the  $\mathcal{Q}_\hbar(J_i)$  are just the usual angular momentum operators.<sup>108</sup>

Mackey's generalization of von Neumann's [1931] uniqueness theorem for the irreducible representations of the canonical commutation relations (1) is his *imprimitivity theorem*. This theorem applies to the special case where  $Q = G/H$  for some (closed) subgroup  $H \subset G$ , and states that (up to unitary equivalence) there is a bijective correspondence between:

1. Systems of imprimitivity  $(\mathcal{H}, U, P)$  for the left-translation of  $G$  on  $G/H$ ;
2. Unitary representations  $U_\chi$  of  $H$ .

This correspondence preserves irreducibility.<sup>109</sup>

<sup>106</sup>For the domain of  $\mathcal{Q}_\hbar(f)$  see footnote 100.

<sup>107</sup>I.e.  $\xi_X^Q f(y) = d/dt|_{t=0}[f(\exp(-tX)y)]$ .

<sup>108</sup>The commutation relations in the previous paragraph are now extended by the familiar relations  $[\mathcal{Q}_\hbar(J_i), \mathcal{Q}_\hbar(J_j)] = i\hbar \epsilon_{ijk} \mathcal{Q}_\hbar(J_k)$ ,  $[\mathcal{Q}_\hbar(J_i), \mathcal{Q}_\hbar(p_j)] = i\hbar \epsilon_{ijk} \mathcal{Q}_\hbar(p_k)$ , and  $[\mathcal{Q}_\hbar(J_i), \mathcal{Q}_\hbar(q^j)] = i\hbar \epsilon_{ijk} \mathcal{Q}_\hbar(q^k)$ .

<sup>109</sup>Specifically, given  $U_\chi$  the triple  $(\mathcal{H}^\chi, U^\chi, P^\chi)$  is a system of imprimitivity, where  $\mathcal{H}^\chi = L^2(G/H) \otimes \mathcal{H}_\chi$  carries the representation  $U^\chi(G)$  induced by  $U_\chi(H)$ , and the  $P^\chi$  act like multiplication operators. Conversely, if  $(\mathcal{H}, U, P)$  is a system of imprimitivity, then there exists a unitary representation  $U_\chi(H)$  such that the triple  $(\mathcal{H}, U, P)$  is unitarily equivalent to the triple  $(\mathcal{H}^\chi, U^\chi, P^\chi)$  just described. For example, for  $G = E(3)$  and  $H = SO(3)$  one has  $\chi = j = 0, 1, 2, \dots$  and  $\mathcal{H}^j = L^2(\mathbb{R}^3) \otimes \mathcal{H}_j$  (where  $\mathcal{H}_j = \mathbb{C}^{2j+1}$  carries the given representation  $U_j(SO(3))$ ).

For example, von Neumann's theorem is recovered as a special case of Mackey's by making the choice  $G = \mathbb{R}^3$  and  $H = \{e\}$  (so that  $Q = \mathbb{R}^3$ , as above): the uniqueness of the (regular) irreducible representation of the canonical commutation relations here follows from the uniqueness of the irreducible representation of the trivial group. A more illustrative example is  $G = E(3)$  and  $H = SO(3)$  (so that  $Q = \mathbb{R}^3$ ), in which case the irreducible representations of the associated system of imprimitivity are classified by spin  $j = 0, 1, \dots$ . Mackey saw this as an explanation for the emergence of spin as a purely quantum-mechanical degree of freedom.<sup>110</sup> Although the opinion that spin has no classical analogue was widely shared also among the pioneers of quantum theory,<sup>111</sup> it is now obsolete (see Subsection 4.3 below). Despite this unfortunate misinterpretation, Mackey's approach to canonical quantization is hard to surpass in power and clarity, and has many interesting applications.<sup>112</sup>

We mention one of specific interest to the philosophy of physics, namely the *Newton–Wigner position operator* (as analyzed by Wightman [1962]).<sup>113</sup> Here the general question is whether a given unitary representation  $U$  of  $G = E(3)$  on some Hilbert space  $\mathcal{H}$  may be extended to a system of imprimitivity with respect to  $H = SO(3)$  (and hence  $Q = \mathbb{R}^3$ , as above); in that case,  $U$  (or rather the associated quantum system) is said to be *localizable* in  $\mathbb{R}^3$ . Following Wigner's (1939) suggestion that a relativistic particle is described by an irreducible representation  $U$  of the Poincaré group  $P$ , one obtains a representation  $U(E(3))$  by restricting  $U(P)$  to the subgroup  $E(3) \subset P$ .<sup>114</sup> It then follows from the previous analysis that the particle described by  $U(P)$  is localizable if and only if  $U(E(3))$  is induced by some representation of  $SO(3)$ . This can, of course, be settled, with the result that massive particles of arbitrary spin can be localized in  $\mathbb{R}^3$  (the corresponding position operator being precisely the one of Newton and Wigner), whereas massless particles may be localized in  $\mathbb{R}^3$  if and only if their helicity is less than one. In particular, the photon (and the graviton) cannot be localized in  $\mathbb{R}^3$  in the stated

<sup>110</sup>By the usual arguments (Wigner's theorem), one may replace  $SO(3)$  by  $SU(2)$ , so as to obtain  $j = 0, 1/2, \dots$

<sup>111</sup>This opinion goes back to Pauli [1925], who talked about a 'klassisch nicht beschreibbare Zweideutigkeit in den quantentheoretischen Eigenschaften des Elektrons,' (i.e. an 'ambivalence in the quantum theoretical properties of the electron that has no classical description') which was later identified as spin by Goudsmit and Uhlenbeck. Probably the first person to draw attention to the classical counterpart of spin was Souriau [1969]. Another misunderstanding about spin is that its ultimate explanation must be found in relativistic quantum mechanics.

<sup>112</sup>This begs the question about the 'best' possible proof of Mackey's imprimitivity theorem. Mackey's own proof was rather measure-theoretic in flavour, and did not shed much light on the origin of his result. Probably the shortest proof has been given by [Ørsted, 1979], but the insight brevity gives is still rather limited. Quite to the contrary, truly transparent proofs reduce a mathematical claim to a tautology. Such proofs, however, tend to require a formidable machinery to make this reduction work; see [Echterhoff *et al.*, 2002] and [Landsman, 2006a] for two different approaches to the imprimitivity theorem in this style.

<sup>113</sup>Fleming and Butterfield [2000] give an up-to-date introduction to particle localization in relativistic quantum theory. See also [De Bièvre, 2003].

<sup>114</sup>Strictly speaking, this hinges on the choice of an inertial frame in Minkowski space, with associated adapted co-ordinates such that the configuration space  $\mathbb{R}^3$  in question is given by  $x^0 = 0$ .

sense.<sup>115</sup>

To appreciate our later material on both phase space quantization and deformation quantization, it is helpful to give a  $C^*$ -algebraic reformulation of Mackey's approach. Firstly, by the spectral theorem [Reed and Simon, 1972; Pedersen, 1989], a projection-valued measure  $E \mapsto P(E)$  on a space  $Q$  taking values in a Hilbert space  $\mathcal{H}$  is equivalent to a nondegenerate representation  $\pi$  of the commutative  $C^*$ -algebra  $C_0(Q)$  on  $\mathcal{H}$  through the correspondence (7).<sup>116</sup> Secondly, if  $\mathcal{H}$  in addition carries a unitary representation  $U$  of  $G$ , the defining condition (4) of a system of imprimitivity (given a  $G$ -action on  $Q$ ) is equivalent to the covariance condition

$$(10) \quad U(x)\mathcal{Q}_\hbar(f)U(x)^{-1} = \mathcal{Q}_\hbar(L_x f)$$

for all  $x \in G$  and  $f \in C_0(Q)$ , where  $L_x f(m) = f(x^{-1}m)$ . Thus a system of imprimitivity for a given  $G$ -action on  $Q$  is "the same" as a covariant nondegenerate representation of  $C_0(Q)$ . Thirdly, from a  $G$ -action on  $Q$  one can construct a certain  $C^*$ -algebra  $C^*(G, Q)$ , the so-called *transformation group  $C^*$ -algebra* defined by the action, which has the property that its nondegenerate representations correspond bijectively (and "naturally") to covariant nondegenerate representations of  $C_0(Q)$ , and therefore to systems of imprimitivity for the given  $G$ -action [Effros and Hahn, 1967; Pedersen, 1979; Landsman, 1998]. In the  $C^*$ -algebraic approach to quantum physics,  $C^*(G, Q)$  is the algebra of observables of a particle moving on  $Q$  subject to the symmetries defined by the  $G$ -action; its inequivalent irreducible representations correspond to the possible superselection sectors of the system [Doebner and Tolar, 1975; Majid, 1988; 1990; Landsman, 1990a; 1990b; 1992].<sup>117</sup>

#### 4.2 Phase space quantization and coherent states

In Mackey's approach to quantization,  $Q$  is the *configuration space* of the system; the associated position coordinates *commute* (cf. (9)). This is reflected by the correspondence just discussed between projection-valued measures on  $Q$  and representations of the *commutative*  $C^*$ -algebra  $C_0(Q)$ . The noncommutativity of observables (and the associated uncertainty relations) typical of quantum mechanics is incorporated by adding the symmetry group  $G$  to the picture and imposing

<sup>115</sup>Seeing photons as quantized light waves with two possible polarizations transverse to the direction of propagation, this last result is physically perfectly reasonable.

<sup>116</sup>A *representation* of a  $C^*$ -algebra  $\mathcal{A}$  on a Hilbert space  $\mathcal{H}$  is a linear map  $\pi : \mathcal{A} \rightarrow \mathcal{B}(\mathcal{H})$  such that  $\pi(AB) = \pi(A)\pi(B)$  and  $\pi(A^*) = \pi(A)^*$  for all  $A, B \in \mathcal{A}$ . Such a representation is called *nondegenerate* when  $\pi(A)\Psi = 0$  for all  $A \in \mathcal{A}$  implies  $\Psi = 0$ .

<sup>117</sup>Another reformulation of Mackey's approach, or rather an extension of it, has been given by Isham [1984]. In an attempt to reduce the whole theory to a problem in group representations, he proposed that the possible quantizations of a particle with configuration space  $G/H$  are given by the inequivalent irreducible representations of a "canonical group"  $G_c = G \ltimes V$ , where  $V$  is the lowest-dimensional vector space that carries a representation of  $G$  under which  $G/H$  is an orbit in the dual vector space  $V^*$ . All pertinent systems of imprimitivity then indeed correspond to unitary representations of  $G_c$ , but this group has many other representations whose physical interpretation is obscure. See also footnote 157.

the relations (4) (or, equivalently, (8) or (10)). As we have pointed out, this procedure upsets the symmetry between the phase space variables position and momentum in classical mechanics.

This somewhat unsatisfactory feature of Mackey's approach may be avoided by replacing  $Q$  by the *phase space* of the system, henceforth called  $M$ .<sup>118</sup> In this approach, noncommutativity is incorporated by a treacherously tiny modification to Mackey's setup. Namely, the projection-valued measure  $E \mapsto P(M)$  on  $M$  with which he starts is now replaced by a *positive-operator-valued measure* or *POVM* on  $M$ , still taking values in some Hilbert space  $\mathcal{K}$ . This is a map  $E \mapsto A(E)$  from the (Borel) subsets  $E$  of  $M$  to the collection of *positive* bounded operators on  $\mathcal{K}$ ,<sup>119</sup> satisfying  $A(\emptyset) = 0$ ,  $A(M) = 1$ , and  $A(\cup_i E_i) = \sum_i A(E_i)$  for any countable collection of disjoint Borel sets  $E_i$ .<sup>120</sup> A POVM that satisfies  $A(E \cap F) = A(E)A(F)$  for all (Borel)  $E, F \subset M$  is precisely a projection-valued measure, so that a POVM is a generalization of the latter.<sup>121</sup> The point, then, is that *a given POVM defines a quantization procedure* by the stipulation that a classical observable  $f$  (i.e. a measurable function on the phase space  $M$ , for simplicity assumed bounded) is quantized by the operator<sup>122</sup>

$$(11) \quad \mathcal{Q}(f) = \int_M dA(x)f(x).$$

Thus the seemingly slight move from projection-valued measures on configuration space to positive-operator valued measures on phase space gives a wholly new perspective on quantization, actually reducing this task to the problem of finding such POVM's.<sup>123</sup>

<sup>118</sup>Here the reader may think of the simplest case  $M = \mathbb{R}^6$ , the space of  $p$ 's and  $q$ 's of a particle moving on  $\mathbb{R}^3$ . More generally, if  $Q$  is the configuration space, the associated phase space is the cotangent bundle  $M = T^*Q$ . Even more general phase spaces, namely arbitrary symplectic manifolds, may be included in the theory as well. References for what follows include [Busch *et al.*, 1998; Schroeck, 1996], and [Landsman, 1998; 1999a].

<sup>119</sup>A bounded operator  $A$  on  $\mathcal{K}$  is called positive when  $(\Psi, A\Psi) \geq 0$  for all  $\Psi \in \mathcal{K}$ . Consequently, it is self-adjoint with spectrum contained in  $\mathbb{R}^+$ .

<sup>120</sup>Here the infinite sum is taken in the weak operator topology. Note that the above conditions force  $0 \leq A(E) \leq 1$ , in the sense that  $0 \leq (\Psi, A(E)\Psi) \leq (\Psi, \Psi)$  for all  $\Psi \in \mathcal{K}$ .

<sup>121</sup>This has given rise to the so-called *operational approach* to quantum theory, in which observables are not represented by self-adjoint operators (or, equivalently, by their associated projection-valued measures), but by POVM's. The space  $M$  on which the POVM is defined is the space of outcomes of the measuring instrument; the POVM is determined by both  $A$  and a calibration procedure for this instrument. The probability that in a state  $\rho$  the outcome of the experiment lies in  $E \subset M$  is taken to be  $\text{Tr}(\rho A(E))$ . See [Davies, 1976; Holevo, 1982; Ludwig, 1985; Schroeck, 1996; Busch *et al.*, 1998], and [De Muynck, 2002].

<sup>122</sup>The easiest way to define the right-hand side of (11) is to fix  $\Psi \in \mathcal{K}$  and define a probability measure  $p_\Psi$  on  $M$  by means of  $p_\Psi(E) = (\Psi, A(E)\Psi)$ . One then *defines*  $\mathcal{Q}(f)$  as an operator through its expectation values  $(\Psi, \mathcal{Q}(f)\Psi) = \int_M dp_\Psi(x)f(x)$ . The expression (11) generalizes (7), and also generalizes the spectral resolution of the operator  $f(A) = \int_{\mathbb{R}} dP(\lambda)f(\lambda)$ , where  $P$  is the projection-valued measure defined by a self-adjoint operator  $A$ .

<sup>123</sup>An important feature of  $\mathcal{Q}$  is that it is *positive* in the sense that if  $f(x) \geq 0$  for all  $x \in M$ , then  $(\Psi, \mathcal{Q}(f)\Psi) \geq 0$  for all  $\Psi \in \mathcal{K}$ . In other words,  $\mathcal{Q}$  is positive as a map from the  $C^*$ -algebra  $C_0(M)$  to the  $C^*$ -algebra  $\mathcal{B}(\mathcal{H})$ .

The solution to this problem is greatly facilitated by *Naimark's dilation theorem*.<sup>124</sup> This states that, given a POVM  $E \mapsto A(E)$  on  $M$  in a Hilbert space  $\mathcal{K}$ , there exists a Hilbert space  $\mathcal{H}$  carrying a projection-valued measure  $P$  on  $M$  and an isometric injection  $\mathcal{K} \hookrightarrow \mathcal{H}$ , such that

$$(12) \quad A(E) = [\mathcal{K}]P(E)[\mathcal{K}]$$

for all  $E \subset M$  (where  $[\mathcal{K}]$  is the orthogonal projection from  $\mathcal{H}$  onto  $\mathcal{K}$ ). Combining this with Mackey's imprimitivity theorem yields a powerful generalization of the latter [Poulsen, 1970; Neumann, 1972; Scutaru, 1977; Cattaneo, 1979; Castrigiano and Henrichs, 1980]. First, define a *generalized system of imprimitivity*  $(\mathcal{K}, U, A)$  for a given action of a group  $G$  on a space  $M$  as a POVM  $A$  on  $M$  taking values in a Hilbert space  $\mathcal{K}$ , along with a unitary representation  $V$  of  $G$  on  $\mathcal{K}$  such that

$$(13) \quad V(x)A(E)V(x)^{-1} = A(xE)$$

for all  $x \in G$  and  $E \subset M$ ; cf. (4). Now assume  $M = G/H$  (and the associated canonical left-action on  $M$ ). The *generalized imprimitivity theorem* states that a generalized system of imprimitivity  $(\mathcal{K}, V, A)$  for this action is necessarily (unitarily equivalent to) a reduction of a system of imprimitivity  $(\mathcal{H}, U, P)$  for the same action. In other words, the Hilbert space  $\mathcal{H}$  in Naimark's theorem carries a unitary representation  $U(G)$  that commutes with the projection  $[\mathcal{K}]$ , and the representation  $V(G)$  is simply the restriction of  $U$  to  $\mathcal{K}$ . Furthermore, the POVM  $A$  has the form (12). The structure of  $(\mathcal{H}, U, P)$  is fully described by Mackey's imprimitivity theorem, so that one has a complete classification of generalized systems of imprimitivity.<sup>125</sup> One has

$$(14) \quad \mathcal{K} = p\mathcal{H}; \quad \mathcal{H} = L^2(M) \otimes \mathcal{H}_\chi,$$

where  $L^2$  is defined with respect to a suitable measure on  $M = G/H$ ,<sup>126</sup> the Hilbert space  $\mathcal{H}_\chi$  carries a unitary representation of  $H$ , and  $p$  is a projection in the commutant of the representation  $U^\chi(G)$  induced by  $U_\chi(G)$ .<sup>127</sup> The quantization (11) is given by

$$(15) \quad \mathcal{Q}(f) = pfp,$$

where  $f$  acts on  $L^2(M) \otimes \mathcal{H}_\chi$  as a multiplication operator, i.e.  $(f\Psi)(x) = f(x)\Psi(x)$ . In particular, one has  $P(E) = \chi_E$  (as a multiplication operator) for a region  $E \subset M$  of phase space, so that  $\mathcal{Q}(\chi_E) = A(E)$ . Consequently, the probability

<sup>124</sup>See, for example, [Riesz and Sz.-Nagy, 1990]. It is better, however, to see Naimark's theorem as a special case of Stinesprings's, as explained e.g. in [Landsman, 1998], and below.

<sup>125</sup>Continuing footnote 109:  $V(G)$  is necessarily a subrepresentation of some representation  $U^\chi(G)$  induced by  $U_\chi(H)$ .

<sup>126</sup>In the physically relevant case that  $G/H$  is symplectic (so that it typically is a coadjoint orbit for  $G$ ) one should take a multiple of the Liouville measure.

<sup>127</sup>The explicit form of  $U^\chi(g)$ ,  $g \in G$ , depends on the choice of a cross-section  $\sigma : G/H \rightarrow G$  of the projection  $\pi : G \rightarrow G/H$  (i.e.  $\pi \circ \sigma = \text{id}$ ). If the measure on  $G/H$  defining  $L^2(G/H)$  is  $G$ -invariant, the explicit formula is  $U^\chi(g)\Psi(x) = U_\chi(s(x)^{-1}gs(g^{-1}x))\Psi(g^{-1}x)$ .

that in a state  $\rho$  (i.e. a density matrix on  $\mathcal{K}$ ) the system is localized in  $E$  is given by  $\text{Tr}(\rho A(E))$ .

In a more natural way than in Mackey’s approach, the covariant POVM quantization method allows one to incorporate space-time symmetries *ab initio* by taking  $G$  to be the Galilei group or the Poincaré group, and choosing  $H$  such that  $G/H$  is a physical phase space (on which  $G$ , then, canonically acts). See [Ali *et al.*, 1995] and [Schroeck, 1996].

Another powerful method of constructing POVM’s on phase space (which in the presence of symmetries overlaps with the preceding one)<sup>128</sup> is based on *coherent states*.<sup>129</sup> The minimal definition of coherent states in a Hilbert space  $\mathcal{H}$  for a phase space  $M$  is that (for some fixed value of Planck’s constant  $\hbar$ , for the moment) one has an injection<sup>130</sup>  $M \hookrightarrow \mathcal{H}$ ,  $z \mapsto \Psi_z^\hbar$ , such that

$$(16) \quad \|\Psi_z^\hbar\| = 1$$

for all  $z \in M$ , and

$$(17) \quad c_\hbar \int_M d\mu_L(z) |(\Psi_z^\hbar, \Phi)|^2 = 1,$$

for each  $\Phi \in \mathcal{H}$  of unit norm (here  $\mu_L$  is the Liouville measure on  $M$  and  $c_\hbar > 0$  is a suitable constant).<sup>131</sup> Condition (17) guarantees that we may define a POVM on  $M$  in  $\mathcal{K}$  by<sup>132</sup>

$$(18) \quad A(E) = c_\hbar \int_E d\mu_L(z) [\Psi_z^\hbar].$$

Eq. (11) then simply reads (inserting the  $\hbar$ -dependence of  $\mathcal{Q}$  and a suffix  $B$  for later use)

$$(19) \quad \mathcal{Q}_\hbar^B(f) = c_\hbar \int_M d\mu_L(z) f(z) [\Psi_z^\hbar].$$

The time-honoured example, due to Schrödinger [1926b], is  $M = \mathbb{R}^{2n}$ ,  $\mathcal{H} = L^2(\mathbb{R}^n)$ , and

$$(20) \quad \Psi_{(p,q)}^\hbar(x) = (\pi\hbar)^{-n/4} e^{-ipq/2\hbar} e^{ipx/\hbar} e^{-(x-q)^2/2\hbar}.$$

<sup>128</sup>Suppose there is a vector  $\Omega \in \mathcal{K}$  such that  $\int_{G/H} d\mu(x) |(\Omega, V(\sigma(x))\Omega)|^2 < \infty$  with respect to some cross-section  $\sigma : G/H \rightarrow G$  and a  $G$ -invariant measure  $\mu$ , as well as  $V(h)\Omega = U_\chi(h)\Omega$  for all  $h \in H$ , where  $U_\chi : H \rightarrow \mathbb{C}$  is *one-dimensional*. Then (taking  $\hbar = 1$ ) the vectors  $V(\sigma(x))\Omega$  (suitably normalized) form a family of coherent states on  $G/H$  [Ali *et al.*, 1995; Schroeck, 1996; Ali, Antoine, and Gazeau, 2000]. For example, the coherent states (20) are of this form for the Heisenberg group.

<sup>129</sup> See [Klauder and Skagerstam, 1985; Perelomov, 1986; Odziejewicz, 1992; Paul and Uribe, 1995; 1996; Ali *et al.*, 1995], and [Ali *et al.*, 2000], for general discussions of coherent states.

<sup>130</sup>This injection must be continuous as a map from  $M$  to  $\mathbb{P}\mathcal{H}$ , the projective Hilbert space of  $\mathcal{H}$ .

<sup>131</sup>Other measures might occur here; see, for example, [Bonechi and De Bièvre, 2000].

<sup>132</sup>Recall that  $[\Psi]$  is the orthogonal projection onto a unit vector  $\Psi$ .

Eq. (17) then holds with  $d\mu_L(p, q) = (2\pi)^{-n}d^npd^nq$  and  $c_{\hbar} = \hbar^{-n}$ . One may verify that  $\mathcal{Q}_{\hbar}^B(p_j)$  and  $\mathcal{Q}_{\hbar}^B(q^j)$  coincide with Schrödinger’s operators (2). This example illustrates that coherent states need *not* be mutually orthogonal; in fact, in terms of  $z = p + iq$  one has for the states in (20)

$$(21) \quad |(\Psi_z^{\hbar}, \Psi_w^{\hbar})|^2 = e^{-|z-w|^2/2\hbar},$$

the significance of this result will emerge later on.

In the general case, it is an easy matter to verify Naimark’s dilation theorem for the POVM (18): changing notation so that the vectors  $\Psi_z^{\hbar}$  now lie in  $\mathcal{K}$ , one finds

$$(22) \quad \mathcal{H} = L^2(M, c_{\hbar}\mu_L),$$

the embedding  $W : \mathcal{K} \hookrightarrow \mathcal{H}$  being given by  $(W\Phi)(z) = (\Psi_z^{\hbar}, \Phi)$ . The projection-valued measure  $P$  on  $\mathcal{H}$  is just  $P(E) = \chi_E$  (as a multiplication operator), and the projection  $p$  onto  $W\mathcal{K}$  is given by

$$(23) \quad p\Psi(z) = c_{\hbar} \int_M d\mu_L(w) (\Psi_z^{\hbar}, \Psi_w^{\hbar}) \Psi(w).$$

Consequently, (19) is unitarily equivalent to (15), where  $f$  acts on  $L^2(M)$  as a multiplication operator.<sup>133</sup>

*Thus (15) and (22) (or its possible extension (14)) form the essence of phase space quantization.*<sup>134</sup>

We close this subsection in the same fashion as the previous one, namely by pointing out the  $C^*$ -algebraic significance of POVM’s. This is extremely easy: whereas a projection-valued measure on  $M$  in  $\mathcal{H}$  is the same as a nondegenerate *representation* of  $C_0(M)$  in  $\mathcal{H}$ , a POVM on  $M$  in a Hilbert space  $\mathcal{K}$  is nothing but a nondegenerate *completely positive map*  $\varphi : C_0(M) \rightarrow \mathcal{B}(\mathcal{K})$ .<sup>135</sup> Consequently, Naimark’s dilation theorem becomes a special case of Stinespring’s [1955] theorem: if  $\mathcal{Q} : \mathcal{A} \rightarrow \mathcal{B}(\mathcal{K})$  is a completely positive map, there exists a Hilbert space  $\mathcal{H}$  carrying a representation  $\pi$  of  $C_0(M)$  and an isometric injection  $\mathcal{K} \hookrightarrow \mathcal{H}$ , such that  $\mathcal{Q}(f) = [\mathcal{K}]\pi(f)[\mathcal{K}]$  for all  $f \in C_0(M)$ . In terms of  $\mathcal{Q}(C_0(M))$ , the covariance condition (13) becomes  $U(x)\mathcal{Q}(f)U(x)^{-1} = \mathcal{Q}(L_x f)$ , just like (10).

<sup>133</sup>This leads to a close relationship between coherent states and Hilbert spaces with a reproducing kernel; see [Landsman, 1998] or [Ali *et al.*, 2000].

<sup>134</sup>See also footnote 172 below.

<sup>135</sup>A map  $\varphi : \mathcal{A} \rightarrow \mathcal{B}$  between  $C^*$ -algebras is called positive when  $\varphi(A) \geq 0$  whenever  $A \geq 0$ ; such a map is called *completely positive* if for all  $n \in \mathbb{N}$  the map  $\varphi_n : \mathcal{A} \otimes M_n(\mathbb{C}) \rightarrow \mathcal{B} \otimes M_n(\mathbb{C})$ , defined by linear extension of  $\varphi \otimes \text{id}$  on elementary tensors, is positive (here  $M_n(\mathbb{C})$  is the  $C^*$ -algebra of  $n \times n$  complex matrices). When  $\mathcal{A}$  is commutative a nondegenerate positive map  $\mathcal{A} \rightarrow \mathcal{B}$  is automatically completely positive for any  $\mathcal{B}$ .



### 4.3 Deformation quantization

So far, we have used the word ‘quantization’ in a heuristic way, basing our account on historical continuity rather than on axiomatic foundations. In this subsection and the next we set the record straight by introducing two alternative ways of looking at quantization in an axiomatic way. We start with the approach that historically came last, but which conceptually is closer to the material just discussed. This is *deformation quantization*, originating in the work of Berezin [1974; 1975a; 1975b], Vey [1975], and Bayen *et al.* [1977]. We here follow the  $C^*$ -algebraic approach to deformation quantization proposed by Rieffel [1989a; 1994], since it is not only mathematically transparent and rigorous, but also reasonably close to physical practice.<sup>136</sup> Due to the mathematical language used, this method of course naturally fits into the general  $C^*$ -algebraic approach to quantum physics.

The key idea of deformation quantization is that quantization should be defined through the property of having the correct classical limit. Consequently, Planck’s “constant”  $\hbar$  is treated as a variable, so that for each of its values one should have a quantum theory. The key requirement is that this family of quantum theories converges to the underlying classical theory as  $\hbar \rightarrow 0$ .<sup>137</sup> The mathematical implementation of this idea is quite beautiful, in that the classical algebra of observables is “glued” to the family of quantum algebras of observables in such a way that the classical theory literally forms the boundary of the space containing the pertinent quantum theories (one for each value of  $\hbar > 0$ ). Technically, this is done through the concept of a *continuous field of  $C^*$ -algebras*.<sup>138</sup> What follows may sound unnecessarily technical, but the last 15 years have indicated that this yields exactly the right definition of quantization.

Let  $I \subset \mathbb{R}$  be the set in which  $\hbar$  takes values; one usually has  $I = [0, 1]$ , but when the phase space is compact,  $\hbar$  often takes values in a countable subset of  $(0, 1]$ .<sup>139</sup> The same situation occurs in the theory of infinite systems; see Section 6. In any case,  $I$  should contain zero as an accumulation point. A continuous field of  $C^*$ -algebras over  $I$ , then, consists of a  $C^*$ -algebra  $\mathcal{A}$ , a collection of  $C^*$ -algebras  $\{\mathcal{A}_\hbar\}_{\hbar \in I}$ , and a surjective morphism  $\varphi_\hbar : \mathcal{A} \rightarrow \mathcal{A}_\hbar$  for each  $\hbar \in I$ , such that:

1. The function  $\hbar \mapsto \|\varphi_\hbar(A)\|_\hbar$  is in  $C_0(I)$  for all  $A \in \mathcal{A}$ ;<sup>140</sup>
2. The norm of any  $A \in \mathcal{A}$  is  $\|A\| = \sup_{\hbar \in I} \|\varphi_\hbar(A)\|$ ;

<sup>136</sup>See also [Landsman, 1998] for an extensive discussion of the  $C^*$ -algebraic approach to deformation quantization. In other approaches to deformation quantization, such as the theory of star products,  $\hbar$  is a formal parameter rather than a real number. In particular, the meaning of the limit  $\hbar \rightarrow 0$  is obscure.

<sup>137</sup>Cf. the preamble to Section 5 for further comments on this limit.

<sup>138</sup>See [Dixmier, 1977; Fell and Doran, 1988], and [Kirchberg and Wassermann, 1995] for three different approaches to the same concept. Our definition follows the latter; replacing  $I$  by an arbitrary locally compact Hausdorff space one finds the general definition.

<sup>139</sup>Cf. [Landsman, 1998] and footnote 204, but in contrast see [Rieffel, 1989a] for the example of the noncommutative torus, where one quantizes a compact phase space for each  $\hbar \in (0, 1]$ . Further examples of this sort are discussed by Natsume and Nest [1999], Natsume, Nest and Ingo [2003], and Hawkins [2005].

<sup>140</sup>Here  $\|\cdot\|_\hbar$  is the norm in the  $C^*$ -algebra  $\mathcal{A}_\hbar$ .

3. For any  $f \in C_0(I)$  and  $A \in \mathcal{A}$  there is an element  $fA \in \mathcal{A}$  for which  $\varphi_{\hbar}(fA) = f(\hbar)\varphi_{\hbar}(A)$  for all  $\hbar \in I$ .

The idea is that the family  $(\mathcal{A}_{\hbar})_{\hbar \in I}$  of  $C^*$ -algebras is glued together by specifying a topology on the bundle  $\coprod_{\hbar \in [0,1]} \mathcal{A}_{\hbar}$  (disjoint union). However, this topology is in fact defined rather indirectly, via the specification of the space of continuous sections of the bundle.<sup>141</sup> Namely, a *continuous section* of the field is *by definition* an element  $\{A_{\hbar}\}_{\hbar \in I}$  of  $\prod_{\hbar \in I} \mathcal{A}_{\hbar}$  (equivalently, a map  $\hbar \mapsto A_{\hbar}$  where  $A_{\hbar} \in \mathcal{A}_{\hbar}$ ) for which there is an  $A \in \mathcal{A}$  such that  $A_{\hbar} = \varphi_{\hbar}(A)$  for all  $\hbar \in I$ . It follows that the  $C^*$ -algebra  $\mathcal{A}$  may actually be identified with the space of continuous sections of the field: if we do so, the morphism  $\varphi_{\hbar}$  is just the evaluation map at  $\hbar$ .<sup>142</sup>

Physically,  $\mathcal{A}_0$  is the commutative algebra of observables of the underlying classical system, and for each  $\hbar > 0$  the noncommutative  $C^*$ -algebra  $\mathcal{A}_{\hbar}$  is supposed to be the algebra of observables of the corresponding quantum system at value  $\hbar$  of Planck’s constant. The algebra  $\mathcal{A}_0$ , then, is of the form  $C_0(M)$ , where  $M$  is the phase space defining the classical theory. A phase space has more structure than an arbitrary topological space; it is a manifold on which a Poisson bracket  $\{, \}$  can be defined. For example, on  $M = \mathbb{R}^{2n}$  one has the familiar expression

$$(24) \quad \{f, g\} = \sum_j \frac{\partial f}{\partial p_j} \frac{\partial g}{\partial q^j} - \frac{\partial f}{\partial q^j} \frac{\partial g}{\partial p_j}.$$

Technically,  $M$  is taken to be a *Poisson manifold*. This is a manifold equipped with a Lie bracket  $\{, \}$  on  $C^\infty(M)$  with the property that for each  $f \in C^\infty(M)$  the map  $g \mapsto \{f, g\}$  defines a derivation of the commutative algebra structure of  $C^\infty(M)$  given by pointwise multiplication. Hence this map is given by a vector field  $\xi_f$ , called the *Hamiltonian vector field* of  $f$  (i.e. one has  $\xi_f g = \{f, g\}$ ). *Symplectic manifolds* are special instances of Poisson manifolds, characterized by the property that the Hamiltonian vector fields exhaust the tangent bundle. A Poisson manifold is foliated by its *symplectic leaves*: a given symplectic leaf  $L$  is characterized by the property that at each  $x \in L$  the tangent space  $T_x L \subset T_x M$  is spanned by the collection of all Hamiltonian vector fields at  $x$ . Consequently, the flow of any Hamiltonian vector field on  $M$  through a given point lies in its entirety within the symplectic leaf containing that point. The simplest example of a Poisson manifold is  $M = \mathbb{R}^{2n}$  with Poisson bracket (24); this manifold is even symplectic.<sup>143</sup>

<sup>141</sup>This is reminiscent of the Gelfand–Naimark theorem for commutative  $C^*$ -algebras, which specifies the topology on a locally compact Hausdorff space  $X$  via the  $C^*$ -algebra  $C_0(X)$ . Similarly, in the theory of (locally trivial) vector bundles the Serre–Swan theorem allows one to reconstruct the topology on a vector bundle  $E \xrightarrow{\pi} X$  from the space  $\Gamma_0(E)$  of continuous sections of  $E$ , seen as a (finitely generated projective)  $C_0(X)$ -module. See, for example, [Gracia-Bondía *et al.*, 2001]. The third condition in our definition of a continuous field of  $C^*$ -algebras makes  $\mathcal{A}$  a  $C_0(I)$ -module in the precise sense that there exists a nondegenerate morphism from  $C_0(I)$  to the center of the multiplier of  $\mathcal{A}$ . This property may also replace our condition 3.

<sup>142</sup>The structure of  $\mathcal{A}$  as a  $C^*$ -algebra corresponds to the operations of pointwise scalar multiplication, addition, adjointing, and operator multiplication on sections.

<sup>143</sup>See [Marsden and Ratiu, 1994] for a mechanics-oriented introduction to Poisson manifolds; also cf. [Landsman, 1998] or [Butterfield, 2005] for the basic facts. A classical mathematical paper on Poisson manifolds is [Weinstein, 1983].

After this preparation, our basic definition is this:<sup>144</sup>

*A deformation quantization of a phase space  $M$  consists of a continuous field of  $C^*$ -algebras  $(\mathcal{A}_\hbar)_{\hbar \in [0,1]}$  (with  $\mathcal{A}_0 = C_0(M)$ ), along with a family of self-adjoint<sup>145</sup> linear maps  $\mathcal{Q}_\hbar : C_c^\infty(M) \rightarrow \mathcal{A}_\hbar$ ,  $\hbar \in (0, 1]$ , such that:*

1. For each  $f \in C_c^\infty(M)$  the map defined by  $0 \mapsto f$  and  $\hbar \mapsto \mathcal{Q}_\hbar(f)$  ( $\hbar \neq 0$ ) is a continuous section of the given continuous field;<sup>146</sup>
2. For all  $f, g \in C_c^\infty(M)$  one has

$$(25) \quad \lim_{\hbar \rightarrow 0} \left\| \frac{i}{\hbar} [\mathcal{Q}_\hbar(f), \mathcal{Q}_\hbar(g)] - \mathcal{Q}_\hbar(\{f, g\}) \right\|_\hbar = 0.$$

Obvious continuity properties one might like to impose, such as

$$(26) \quad \lim_{\hbar \rightarrow 0} \|\mathcal{Q}_\hbar(f)\mathcal{Q}_\hbar(g) - \mathcal{Q}_\hbar(fg)\| = 0,$$

or

$$(27) \quad \lim_{\hbar \rightarrow 0} \|\mathcal{Q}_\hbar(f)\| = \|f\|_\infty,$$

turn out to be an automatic consequence of this definition.<sup>147</sup> Condition (25), however, transcends the  $C^*$ -algebraic setting, and is the key ingredient in proving (among other things) that the quantum dynamics converges to the classical dynamics;<sup>148</sup> see Section 5. The map  $\mathcal{Q}_\hbar$  is the quantization map at value  $\hbar$  of Planck's constant; we feel it is the most precise formulation of Heisenberg's original *Umdeutung* of classical observables known to date. It has the same interpretation as the heuristic symbol  $\mathcal{Q}_\hbar$  used so far: the operator  $\mathcal{Q}_\hbar(f)$  is the quantum-mechanical observable whose classical counterpart is  $f$ .

This has turned out to be an fruitful definition of quantization, firstly because most well-understood examples of quantization fit into it [Rieffel, 1994; Landsman, 1998], and secondly because it has suggested various fascinating new ones [Rieffel,

<sup>144</sup>Here  $C_c^\infty(M)$  stands for the space of smooth functions on  $M$  with compact support; this is a norm-dense subalgebra of  $\mathcal{A}_0 = C_0(M)$ . The question whether the maps  $\mathcal{Q}_\hbar$  can be extended from  $C_c^\infty(M)$  to  $C_0(M)$  has to be answered on a case by case basis. Upon such an extension, if it exists, condition (25) will lose its meaning, since the Poisson bracket  $\{f, g\}$  is not defined for all  $f, g \in C_0(M)$ .

<sup>145</sup>I.e.  $\mathcal{Q}_\hbar(\bar{f}) = \mathcal{Q}_\hbar(f)^*$ .

<sup>146</sup>Equivalently, one could extend the family  $(\mathcal{Q}_\hbar)_{\hbar \in (0,1]}$  to  $\hbar = 0$  by  $\mathcal{Q}_0 = \text{id}$ , and state that  $\hbar \mapsto \mathcal{Q}_\hbar(f)$  is a continuous section. Also, one could replace this family of maps by a single section  $\mathcal{Q} : C_c^\infty(M) \rightarrow \mathcal{A}$  of  $\varphi_0$  and define  $\mathcal{Q}_\hbar = \varphi_\hbar \circ \mathcal{Q} : C_c^\infty(M) \rightarrow \mathcal{A}_\hbar$ .

<sup>147</sup>That they are automatic should not distract from the fact that especially (27) is a beautiful connection between classical and quantum mechanics. See footnote 89 for the meaning of  $\|f\|_\infty$ .

<sup>148</sup>This insight is often attributed to Dirac [1930], who was the first to recognize the analogy between the commutator in quantum mechanics and the Poisson bracket in classical mechanics. In fact, the Poisson structure on  $M$  is uniquely determined by the continuous field structure together with condition (25). Thus the choice of the  $\mathcal{Q}_\hbar$  is secondary.

1989a; Natsume and Nest, 1999; Natsume *et al.*, 2003; Hawkins, 2005]. Restricting ourselves to the former, we note, for example, that (19) with (20) defines a deformation quantization of the phase space  $\mathbb{R}^{2n}$  (with standard Poisson bracket) if one takes  $\mathcal{A}_\hbar$  to be the  $C^*$ -algebra of compact operators on the Hilbert space  $L^2(\mathbb{R}^n)$ . This is called the *Berezin quantization* of  $\mathbb{R}^{2n}$  (as a phase space);<sup>149</sup> explicitly, for  $\Phi \in L^2(\mathbb{R}^n)$  one has

$$(28) \quad \mathcal{Q}_\hbar^B(f)\Phi(x) = \int_{\mathbb{R}^{2n}} \frac{d^n p d^n q d^n y}{(2\pi\hbar)^n} f(p, q) \overline{\Psi_{(p,q)}^\hbar(y)} \Phi(y) \Psi_{(p,q)}^\hbar(x).$$

This quantization has the distinguishing feature of positivity,<sup>150</sup> a property not shared by its more famous sister called *Weyl quantization*.<sup>151</sup> The latter is a deformation quantization of  $\mathbb{R}^{2n}$  as well, having the same continuous field of  $C^*$ -algebras, but differing from Berezin quantization in its quantization map

$$(29) \quad \mathcal{Q}_\hbar^W(f)\Phi(x) = \int_{\mathbb{R}^{2n}} \frac{d^n p d^n q}{(2\pi\hbar)^n} e^{ip(x-q)/\hbar} f(p, \frac{1}{2}(x+q)) \Phi(q).$$

Although it lacks good positivity and hence continuity properties,<sup>152</sup> Weyl quantization enjoys better symmetry properties than Berezin quantization.<sup>153</sup> Despite these differences, which illustrate the lack of uniqueness of concrete quantization procedures, Weyl and Berezin quantization both reproduce Schrödinger’s position and momentum operators (2).<sup>154</sup> Furthermore, if  $f \in L^1(\mathbb{R}^{2n})$ , then  $\mathcal{Q}_\hbar^B(f)$  and  $\mathcal{Q}_\hbar^W(f)$  are trace class, with

$$(30) \quad \text{Tr } \mathcal{Q}_\hbar^B(f) = \text{Tr } \mathcal{Q}_\hbar^W(f) = \int_{\mathbb{R}^{2n}} \frac{d^n p d^n q}{(2\pi\hbar)^n} f(p, q).$$

Weyl and Berezin quantization are related by

$$(31) \quad \mathcal{Q}_\hbar^B(f) = \mathcal{Q}_\hbar^W(e^{\frac{\hbar}{4}\Delta_{2n}} f),$$

<sup>149</sup>In the literature, Berezin quantization on  $\mathbb{R}^{2n}$  is often called anti-Wick quantization (or ordering), whereas on compact complex manifolds it is sometimes called Toeplitz or Berezin–Toeplitz quantization. Coherent states based on other phase spaces often define deformation quantizations as well; see [Landsman, 1998].

<sup>150</sup>Cf. footnote 123. As a consequence, (28) is valid not only for  $f \in C_c^\infty(\mathbb{R}^{2n})$ , but even for all  $f \in L^\infty(\mathbb{R}^{2n})$ , and the extension of  $\mathcal{Q}_\hbar^B$  from  $C_c^\infty(\mathbb{R}^{2n})$  to  $L^\infty(\mathbb{R}^{2n})$  is continuous.

<sup>151</sup>The original reference is Weyl [1931]. See, for example, [Dubin *et al.*, 2000] and [Esposito *et al.*, 2004] for a modern physics-oriented yet mathematically rigorous treatment. See also [Rieffel, 1994] and [Landsman, 1998] for a discussion from the perspective of deformation quantization, as well as [Binz *et al.*, 2004] for infinite-dimensional examples.

<sup>152</sup>Nonetheless, Weyl quantization may be extended from  $C_c^\infty(\mathbb{R}^{2n})$  to much larger function spaces using techniques from the theory of distributions (leaving the Hilbert space setting typical of quantum mechanics). The classical treatment is in Hörmander [1979; 1985a].

<sup>153</sup>Weyl quantization is covariant under the affine symplectic group  $\text{Sp}(n, \mathbb{R}) \ltimes \mathbb{R}^{2n}$ , whereas Berezin quantization is merely covariant under its subgroup  $\text{O}(2n) \ltimes \mathbb{R}^{2n}$ .

<sup>154</sup>This requires a formal extension of the maps  $\mathcal{Q}_\hbar^W$  and  $\mathcal{Q}_\hbar^B$  to unbounded functions on  $M$  like  $p_j$  and  $q^j$ .

where  $\Delta_{2n} = \sum_{j=1}^n (\partial^2/\partial p_j^2 + \partial^2/\partial(q^j)^2)$ , from which it may be shown that Weyl and Berezin quantization are *asymptotically equal* in the sense that for any  $f \in C_c^\infty(\mathbb{R}^{2n})$  one has

$$(32) \quad \lim_{\hbar \rightarrow 0} \|\mathcal{Q}_\hbar^B(f) - \mathcal{Q}_\hbar^W(f)\| = 0.$$

Mackey’s approach to quantization also finds its natural home in the setting of deformation quantization. Let a Lie group  $G$  act on a manifold  $Q$ , interpreted as a *configuration space*, as in Subsection 4.1. It turns out that the corresponding classical *phase space* is the manifold  $\mathfrak{g}^* \times Q$ , equipped with the so-called *semidirect product Poisson structure* [Marsden *et al.*, 1984; Krishnaprasad and Marsden, 1987]. Relative to a basis  $(T_a)$  of the Lie algebra  $\mathfrak{g}$  of  $G$  with structure constants  $C_{ab}^c$  (i.e.  $[T_a, T_b] = \sum_c C_{ab}^c T_c$ ), the Poisson bracket in question is given by

$$(33) \quad \{f, g\} = \sum_a \left( \xi_a^M f \frac{\partial g}{\partial \theta_a} - \frac{\partial f}{\partial \theta_a} \xi_a^M g \right) - \sum_{a,b,c} C_{ab}^c \theta_c \frac{\partial f}{\partial \theta_a} \frac{\partial g}{\partial \theta_b},$$

where  $\xi_a^M = \xi_{T_a}^M$ . To illustrate the meaning of this lengthy expression, we consider a few special cases. First, take  $f = X \in \mathfrak{g}$  and  $g = Y \in \mathfrak{g}$  (seen as linear functions on the dual  $\mathfrak{g}^*$ ). This yields

$$(34) \quad \{X, Y\} = -[X, Y].$$

Subsequently, assume that  $g$  depends on position  $q$  alone. This leads to

$$(35) \quad \{X, g\} = -\xi_X^M g.$$

Finally, assume that  $f = f_1$  and  $g = f_2$  depend on  $q$  only; this clearly gives

$$(36) \quad \{f_1, f_2\} = 0.$$

The two simplest physically relevant examples, already considered at the quantum level in Subsection 4.1, are as follows. First, take  $G = \mathbb{R}^n$  (as a Lie group) and  $Q = \mathbb{R}^n$  (as a manifold), with  $G$  acting on  $Q$  by translation. Eqs. (34) - (36) then yield the Poisson brackets  $\{p_j, p_k\} = 0$ ,  $\{p_j, q^k\} = \delta_j^k$ , and  $\{q^j, q^k\} = 0$ , showing that in this case  $M = \mathfrak{g}^* \times Q = \mathbb{R}^{2n}$  is the standard phase space of a particle moving in  $\mathbb{R}^n$ ; cf. (24). Second, the case  $G = E(3)$  and  $Q = \mathbb{R}^3$  yields a phase space  $M = \mathbb{R}^3 \times \mathbb{R}^6$ , where  $\mathbb{R}^6$  is the phase space of a spinless particle just considered, and  $\mathbb{R}^3$  is an additional internal space containing spin as a classical degree of freedom. Indeed, beyond the Poisson brackets on  $\mathbb{R}^6$  just described, (34) - (36) give rise to the additional Poisson brackets  $\{J_i, J_j\} = \epsilon_{ijk} J_k$ ,  $\{J_i, p_j\} = \epsilon_{ijk} p_k$ , and  $\{J_i, q^j\} = \epsilon_{ijk} q^k$ .<sup>155</sup>

The analogy between (34), (35), (36) on the one hand, and (6), (8), (9), respectively, on the other, is no accident: the Poisson brackets in question *are* the

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<sup>155</sup>These are the classical counterparts of the commutation relations for angular momentum written down in footnote 108.

classical counterpart of the commutation relations just referred to. This observation is made precise by the fundamental theorem relating Mackey’s systems of imprimitivity to deformation quantization [Landsman, 1993; 1998]: one can equip the family of  $C^*$ -algebras

$$(37) \quad \begin{aligned} \mathcal{A}_0 &= C_0(\mathfrak{g}^* \times Q); \\ \mathcal{A}_{\hbar} &= C^*(G, Q), \end{aligned}$$

where  $C^*(G, Q)$  is the transformation group  $C^*$ -algebra defined by the given  $G$ -action on  $Q$  (cf. the end of Subsection 4.1), with the structure of a continuous field, and one can define quantization maps  $\mathcal{Q}_{\hbar} : C_c^\infty(\mathfrak{g}^* \times Q) \rightarrow C^*(G, Q)$  so as to obtain a deformation quantization of the phase space  $\mathfrak{g}^* \times Q$ . It turns out that for special functions of the type  $X, Y \in \mathfrak{g}$ , and  $f = f(q)$  just considered, the equality

$$(38) \quad \frac{i}{\hbar} [\mathcal{Q}_{\hbar}(f), \mathcal{Q}_{\hbar}(g)] - \mathcal{Q}_{\hbar}(\{f, g\}) = 0$$

holds exactly (and not merely asymptotically for  $\hbar \rightarrow 0$ , as required in the fundamental axiom (25) for deformation quantization).

This result clarifies the status of Mackey’s quantization by systems of imprimitivity. The classical theory underlying the relations (4) is not the usual phase space  $T^*Q$  of a structureless particle moving on  $Q$ , but  $M = \mathfrak{g}^* \times Q$ . For simplicity we restrict ourselves to the transitive case  $Q = G/H$  (with canonical left  $G$ -action). Then  $M$  coincides with  $T^*Q$  only when  $H = \{e\}$  and hence  $Q = G$ ; <sup>156</sup> in general, the phase space  $\mathfrak{g}^* \times (G/H)$  is *locally* of the form  $T^*(G/H) \times \mathfrak{h}^*$  (where  $\mathfrak{h}^*$  is the dual of the Lie algebra of  $H$ ). The internal degree of freedom described by  $\mathfrak{h}^*$  is a generalization of classical spin, which, as we have seen, emerges in the case  $G = E(3)$  and  $H = SO(3)$ . All this is merely a special case of a vast class of deformation quantizations described by Lie groupoids; see [Landsman, 1998; 1999b; 2006a] and [Landsman and Ramazan, 2001]. <sup>157</sup>

#### 4.4 Geometric quantization

Because of its use of abstract  $C^*$ -algebras, deformation quantization is a fairly sophisticated and recent technique. Historically, it was preceded by a more concrete and traditional approach called *geometric quantization*. <sup>158</sup> Here the goal is to

<sup>156</sup>For a Lie group  $G$  one has  $T^*G \cong \mathfrak{g}^* \times G$ .

<sup>157</sup>A similar analysis can be applied to Isham’s [1984] quantization scheme mentioned in footnote 117. The unitary irreducible representations of the canonical group  $G_c$  stand in bijective correspondence with the nondegenerate representations of the group  $C^*$ -algebra  $C^*(G_c)$  [Pedersen, 1979], which is a deformation quantization of the Poisson manifold  $\mathfrak{g}_c^*$  (i.e. the dual of the Lie algebra of  $G_c$ ). This Poisson manifold contains the coadjoint orbits of  $G_c$  as “irreducible” classical phase spaces, of which only one is the cotangent bundle  $T^*(G/H)$  one initially thought one was quantizing (see [Landsman, 1998] for the classification of the coadjoint orbits of semidirect products). All other orbits are mere lumber that one should avoid. See also [Robson, 1996]. If one is ready for groupoids, there is no need for the canonical group approach.

<sup>158</sup>Geometric quantization was independently introduced by Kostant [1970] and Souriau [1969]. Major later treatments on the basis of the original formalism are [Guillemin and Sternberg, 1977;

firstly “quantize” a phase space  $M$  by a concretely given Hilbert space  $\mathcal{H}(M)$ , and secondly to map the classical observables (i.e. the real-valued smooth functions on  $M$ ) into self-adjoint operators on  $\mathcal{H}$  (which after all play the role of observables in von Neumann’s formalism of quantum mechanics).<sup>159</sup> In principle, this program should align geometric quantization much better with the fundamental role unbounded self-adjoint operators play in quantum mechanics than deformation quantization, but in practice geometric quantization continues to be plagued by problems.<sup>160</sup> However, it would be wrong to see deformation quantization and geometric quantization as *competitors*; as we shall see in the next subsection, they are natural *allies*, forming “complementary” parts of a conjectural quantization functor.

In fact, in our opinion geometric quantization is best compared and contrasted with phase space quantization in its concrete formulation of Subsection 4.2 (i.e. before its  $C^*$ -algebraic abstraction and subsequent absorption into deformation quantization as indicated in Subsection 4.3).<sup>161</sup> For geometric quantization equally well starts with the Hilbert space  $L^2(M)$ ,<sup>162</sup> and subsequently attempts to construct  $\mathcal{H}(M)$  from it, though typically in a different way from (14).

Before doing so, however, the geometric quantization procedure first tries to define a linear map  $\mathcal{Q}_\hbar^{pre}$  from  $C^\infty(M)$  to the class of (generally unbounded) operators on  $L^2(M)$  that formally satisfies

$$(39) \quad \frac{i}{\hbar}[\mathcal{Q}_\hbar^{pre}(f), \mathcal{Q}_\hbar^{pre}(g)] - \mathcal{Q}_\hbar^{pre}(\{f, g\}) = 0,$$

i.e. (38) with  $\mathcal{Q} = \mathcal{Q}_\hbar^{pre}$ , as well as the nondegeneracy property

$$(40) \quad \mathcal{Q}_\hbar^{pre}(\chi_M) = 1,$$

where  $\chi_M$  is the function on  $M$  that is identically equal to 1, and the 1 on the right-hand side is the unit operator on  $L^2(M)$ . Such a map is called a *prequantization*

Śniatycki, 1980; Kirillov, 1990; Woodhouse, 1992; Puta, 1993; Chernoff, 1995; Kirillov, 2004], and [Ali and Englis, 2004]. The modern era (based on the use of Dirac operators and  $K$ -theory) was initiated by unpublished remarks by Bott in the early 1990s; see [Vergne, 1994] and [Guillemin *et al.*, 2002]. The postmodern (i.e. functorial) epoch was launched in [Landsman, 2005].

<sup>159</sup>In geometric quantization phase spaces are always seen as symplectic manifolds (with the sole exception of [Vaisman, 1991]; the reason why it is unnatural to start with the more general class of Poisson manifolds will become clear in the next subsection.

<sup>160</sup>Apart from rather technical issues concerning the domains and self-adjointness properties of the operators defined by geometric quantization, the main point is that the various mathematical choices one has to make in the geometric quantization procedure cannot all be justified by physical arguments, although the physical properties of the theory depend on these choices. (The notion of a polarization is the principal case in point; see also footnote 173 below.) Furthermore, as we shall see, one cannot quantize sufficiently many functions in standard geometric quantization. Our functorial approach to geometric quantization in Subsection 4.5 was partly invented to alleviate these problems.

<sup>161</sup>See also [Tuynman, 1987].

<sup>162</sup>Defined with respect to the Liouville measure times a suitable factor  $c_\hbar$ , as in (17) etc.; in geometric quantization this factor is not very important, as it is unusual to study the limit  $\hbar \rightarrow 0$ . For  $M = \mathbb{R}^{2n}$  the measure on  $M$  with respect to which  $L^2(M)$  is defined is  $d^n p d^n q / (2\pi\hbar)^n$ .

of  $M$ .<sup>163</sup> For  $M = \mathbb{R}^{2n}$  (equipped with its standard Poisson bracket (24)), a prequantization map is given (on  $\Phi \in L^2(M)$ ) by

$$(41) \quad \mathcal{Q}_\hbar^{pre}(f)\Phi = -i\hbar\{f, \Phi\} + \left( f - \sum_j p_j \frac{\partial f}{\partial p_j} \right) \Phi.$$

This expression is initially defined for  $\Phi \in C_c^\infty(M) \subset L^2(M)$ , on which domain  $\mathcal{Q}_\hbar^{pre}(f)$  is symmetric when  $f$  is real-valued;<sup>164</sup> note that the operator in question is unbounded even when  $f$  is bounded.<sup>165</sup> This looks complicated; the simpler expression  $\mathcal{Q}_\hbar(f)\Phi = -i\hbar\{f, \Phi\}$ , however, would satisfy (38) but not (40), and the goal of the second term in (41) is to satisfy the latter condition while preserving the former.<sup>166</sup> For example, one has

$$(42) \quad \begin{aligned} \mathcal{Q}_\hbar^{pre}(q^k) &= q^k + i\hbar \frac{\partial}{\partial p_k}; \\ \mathcal{Q}_\hbar^{pre}(p_j) &= -i\hbar \frac{\partial}{\partial q^j}. \end{aligned}$$

For general phase spaces  $M$  one may construct a map  $\mathcal{Q}_\hbar^{pre}$  that satisfies (39) and (40) when  $M$  is “prequantizable”; a full explanation of this notion requires some differential geometry.<sup>167</sup> Assuming this to be the case, then for one thing prequantization is a very effective tool in constructing unitary group representations of the kind that are interesting for physics. Namely, suppose a Lie group  $G$  acts on the phase space  $M$  in “canonical” fashion. This means that there exists a map  $\mu : M \rightarrow \mathfrak{g}^*$ , called the *momentum map*, such that  $\xi_{\mu_X} = \xi_X^M$  for each

<sup>163</sup>The idea of prequantization predates geometric quantization; see [van Hove, 1951] and [Segal, 1960].

<sup>164</sup>An operator  $A$  defined on a dense subspace  $\mathcal{D} \subset \mathcal{H}$  of a Hilbert space  $\mathcal{H}$  is called *symmetric* when  $(A\Psi, \Phi) = (\Psi, A\Phi)$  for all  $\Psi, \Phi \in \mathcal{D}$ .

<sup>165</sup>As mentioned, self-adjointness is a problem in geometric quantization; we will not address this issue here. Berezin quantization is much better behaved than geometric quantization in this respect, since it maps bounded functions into bounded operators.

<sup>166</sup>One may criticize the geometric quantization procedure for emphasizing (39) against its equally natural counterpart  $\mathcal{Q}(fg) = \mathcal{Q}(f)\mathcal{Q}(g)$ , which fails to be satisfied by  $\mathcal{Q}_\hbar^{pre}$  (and indeed by any known quantization procedure, except the silly  $\mathcal{Q}(f) = f$  (as a multiplication operator on  $L^2(M)$ )).

<sup>167</sup>A symplectic manifold  $(M, \omega)$  is called *prequantizable* at some fixed value of  $\hbar$  when it admits a complex line bundle  $L \rightarrow M$  (called the *prequantization line bundle*) with connection  $\nabla$  such that  $F = -i\omega/\hbar$  (where  $F$  is the curvature of the connection, defined by  $F(X, Y) = [\nabla_X, \nabla_Y] - \nabla_{[X, Y]}$ ). This is the case iff  $[\omega]/2\pi\hbar \in H^2(M, \mathbb{Z})$ , where  $[\omega]$  is the de Rham cohomology class of the symplectic form. If so, prequantization is defined by the formula  $\mathcal{Q}_\hbar^{pre}(f) = -i\hbar\nabla_{\xi_f} + f$ , where  $\xi_f$  is the Hamiltonian vector field of  $f$  (see Subsection 4.3). This expression is defined and symmetric on the space  $C_c^\infty(M, L) \subset L^2(M)$  of compactly supported smooth sections of  $L$ , and is easily checked to satisfy (39) and (40). To obtain (41) as a special case, note that for  $M = \mathbb{R}^{2n}$  with the canonical symplectic form  $\omega = \sum_k dp_k \wedge dq^k$  one has  $[\omega] = 0$ , so that  $L$  is the trivial bundle  $L = \mathbb{R}^{2n} \times \mathbb{C}$ . The connection  $\nabla = d + A$  with  $A = -\frac{i}{\hbar} \sum_k p_k dq^k$  satisfies  $F = -i\omega/\hbar$ , and this eventually yields (41).



$X \in \mathfrak{g}$ ,<sup>168</sup> and in addition  $\{\mu_X, \mu_Y\} = \mu_{[X, Y]}$ . See [Abraham and Marsden, 1985; Marsden and Ratiu, 1994; Landsman, 1998; Belot, 2005; Butterfield, 2005], etc. On then obtains a representation  $\pi$  of the Lie algebra  $\mathfrak{g}$  of  $G$  by skew-symmetric unbounded operators on  $L^2(M)$  through

$$(43) \quad \pi(X) = -i\hbar \mathcal{Q}_\hbar^{pre}(\mu_X),$$

which often exponentiates to a unitary representation of  $G$ .<sup>169</sup>

As the name suggests, prequantization is not yet quantization. For example, the prequantization of  $M = \mathbb{R}^{2n}$  does not reproduce Schrödinger's wave mechanics: the operators (42) are not unitarily equivalent to (2). In fact, as a carrier of the representation (42) of the canonical commutation relations (1), the Hilbert space  $L^2(\mathbb{R}^{2n})$  contains  $L^2(\mathbb{R}^n)$  (carrying the representation (2)) with infinite multiplicity [Ali and Emch, 1986]. This situation is often expressed by the statement that "prequantization is reducible" or that the prequantization Hilbert space  $L^2(M)$  is 'too large', but both claims are misleading:  $L^2(M)$  is actually *irreducible* under the action of  $\mathcal{Q}_\hbar^{pre}(C^\infty(M))$  [Tuynman, 1998], and saying that for example  $L^2(\mathbb{R}^n)$  is "larger" than  $L^2(\mathbb{R}^n)$  is unmathematical in view of the unitary isomorphism of these Hilbert spaces. What is really meant here is that in typical examples  $L^2(M)$  is generically reducible under the action of some Lie algebra where one would like it to be irreducible. This applies, for example, to (2), which defines a representation of the Lie algebra of the Heisenberg group. More generally, in the case where a phase space  $M$  carries a transitive action of a Lie group  $G$ , so that one would expect the quantization of this  $G$ -action by unitary operators on a Hilbert space to be irreducible,  $L^2(M)$  is typically highly reducible under the representation (43) of  $\mathfrak{g}$ .<sup>170</sup>

Phase space quantization encounters this problem as well. Instead of the complicated expression (41), through (11) it simply "phase space prequantizes"  $f \in C^\infty(M)$  on  $L^2(M)$  by  $f$  as a multiplication operator.<sup>171</sup> Under this action of  $C^\infty(M)$  the Hilbert space  $L^2(M)$  is of course highly reducible.<sup>172</sup> The identifica-

<sup>168</sup>Here  $\mu_X \in C^\infty(M)$  is defined by  $\mu_X(x) = \langle \mu(x), X \rangle$ , and  $\xi_X^M$  is the vector field on  $M$  defined by the  $G$ -action (cf. footnote 107). Hence this condition means that  $\{\mu_X, f\}(y) = d/dt|_{t=0}[f(\exp(-tX)y)]$  for all  $f \in C^\infty(M)$  and all  $y \in M$ .

<sup>169</sup>An operator  $A$  defined on a dense subspace  $\mathcal{D} \subset \mathcal{H}$  of a Hilbert space  $\mathcal{H}$  is called *skew-symmetric* when  $(A\Psi, \Phi) = -(\Psi, A\Phi)$  for all  $\Psi, \Phi \in \mathcal{D}$ . If one has a unitary representation  $U$  of a Lie group  $G$  on  $\mathcal{H}$ , then the derived representation  $dU$  of the Lie algebra  $\mathfrak{g}$  (see footnote 104) consists of skew-symmetric operators, making one hopeful that a given representation of  $\mathfrak{g}$  by skew-symmetric operators can be integrated (or exponentiated) to a unitary representation of  $G$ . See [Barut and Račka, 1977] or [Jørgensen and Moore, 1984] and references therein.

<sup>170</sup>This can be made precise in the context of the so-called orbit method, cf. the books cited in footnote 158.

<sup>171</sup>For unbounded  $f$  this operator is defined on the set of all  $\Phi \in L^2(M)$  for which  $f\Phi \in L^2(M)$ .

<sup>172</sup>Namely, each (measurable) subset  $E \subset M$  defines a projection  $\chi_E$ , and  $\chi_E L^2(M)$  is stable under all multiplication operators  $f$ . One could actually decide not to be bothered by this problem and stop here, but then one is simply doing classical mechanics in a Hilbert space setting [Koopman, 1931]. This formalism even turns out to be quite useful for ergodic theory [Reed and Simon, 1972].

tion of an appropriate subspace

$$(44) \quad \mathcal{H}(M) = pL^2(M)$$

of  $L^2(M)$  (where  $p$  is a projection) as the Hilbert space carrying the “quantization” of  $M$  (or rather of  $C^\infty(M)$ ) may be seen as a solution to this reducibility problem, for if the procedure is successful, the projection  $p$  is chosen such that  $pL^2(M)$  is irreducible under  $pC^\infty(M)p$ . Moreover, in this way practically any function on  $M$  can be quantized, albeit at the expense of (38) (which, as we have seen, gets replaced by its asymptotic version (25)). See Subsection 6.3 for a discussion of reducibility versus irreducibility of representations of algebras of observables in classical and quantum theory.

We restrict our treatment of geometric quantization to situations where it adopts the same strategy as above, in assuming that the final Hilbert space has the form (44) as well.<sup>173</sup> But it crucially differs from phase space quantization in that its first step is (41) (or its generalization to more general phase spaces) rather than just having  $f\Phi$  on the right-hand side.<sup>174</sup> Moreover, in geometric quantization one merely quantizes a *subspace* of the set  $C^\infty(M)$  of classical observables, consisting of those functions that satisfy

$$(45) \quad [\mathcal{Q}_\hbar^{pre}(f), p] = 0.$$

If a function  $f \in C^\infty(M)$  satisfies this condition, then one defines the “geometric quantization” of  $f$  as

$$(46) \quad \mathcal{Q}_\hbar^G(f) = \mathcal{Q}_\hbar^{pre}(f) \upharpoonright \mathcal{H}(M).$$

This is well defined, since because of (45) the operator  $\mathcal{Q}_\hbar^{pre}(f)$  now maps  $pL^2(M)$  onto itself. Hence (38) holds for  $\mathcal{Q}_\hbar = \mathcal{Q}_\hbar^G$  because of (39); in geometric quantization one simply refuses to quantize functions for which (38) is *not* valid.

Despite some impressive initial triumphs,<sup>175</sup> there is no general method that accomplishes the goals of geometric quantization with guaranteed success. Therefore, geometric quantization has remained something like a hacker’s tool, whose applicability largely depends on the creativity of the user.

In any case, our familiar example  $M = \mathbb{R}^{2n}$  is well understood, and we illustrate the general spirit of the method in its setting, simplifying further by taking  $n = 1$ . It is convenient to replace the canonical coordinates  $(p, q)$  on  $M$  by  $z = p + iq$  and  $\bar{z} = p - iq$ , and the mathematical toolkit of geometric quantization makes it very

<sup>173</sup> Geometric quantization has traditionally been based on the notion of a polarization (cf. the references in footnote 158). This device produces a final Hilbert space  $\mathcal{H}(M)$  which may not be a subspace of  $L^2(M)$ , except in the so-called (anti-) holomorphic case.

<sup>174</sup>It also differs from phase space quantization in the ideology that the projection  $p$  ought to be constructed solely from the geometry of  $M$ : hence the name ‘geometric quantization’.

<sup>175</sup>Such as the orbit method for nilpotent groups and the newly understood Borel–Weil method for compact groups, cf. [Kirillov, 2004] and most other books cited in footnote 158.

natural to look at the space of solutions within  $L^2(\mathbb{R}^2)$  of the equations<sup>176</sup>

$$(47) \quad \left( \frac{\partial}{\partial \bar{z}} + \frac{z}{4\hbar} \right) \Phi(z, \bar{z}) = 0.$$

The general solution of these equations that lies in  $L^2(\mathbb{R}^2) = L^2(\mathbb{C})$  is

$$(48) \quad \Phi(z, \bar{z}) = e^{-|z|^2/4\hbar} f(z),$$

where  $f$  is a holomorphic function such that

$$(49) \quad \int_{\mathbb{C}} \frac{dz d\bar{z}}{2\pi\hbar i} e^{-|z|^2/2\hbar} |f(z)|^2 < \infty.$$

The projection  $p$ , then, is the projection onto the closed subspace of  $L^2(\mathbb{C})$  consisting of these solutions.<sup>177</sup> The Hilbert space  $pL^2(\mathbb{C})$  is unitarily equivalent to  $L^2(\mathbb{R})$  in a natural way (i.e. without the choice of a basis). The condition (45) boils down to  $\partial^2 f(z, \bar{z})/\partial \bar{z}_i \partial \bar{z}_j = 0$ ; in particular, the coordinate functions  $q$  and  $p$  are quantizable. Transforming to  $L^2(\mathbb{R})$ , one finds that the operators  $\mathcal{Q}_\hbar^G(q)$  and  $\mathcal{Q}_\hbar^G(p)$  coincide with Schrödinger’s expressions (2). In particular, the Heisenberg group  $H_1$ , which acts with infinite multiplicity on  $L^2(\mathbb{C})$ , acts irreducibly on  $pL^2(\mathbb{C})$ .

#### 4.5 Epilogue: functoriality of quantization

A very important aspect of quantization is its interplay with symmetries and constraints. Indeed, the fundamental theories describing Nature (viz. electrodynamics, Yang–Mills theory, general relativity, and possibly also string theory) are a priori formulated as constrained systems. The classical side of constraints and reduction is well understood,<sup>178</sup> a large class of important examples being codified by the procedure of symplectic reduction. A special case of this is *Marsden–Weinstein reduction*: if a Lie group  $G$  acts on a phase space  $M$  in canonical fashion with momentum map  $\mu : M \rightarrow \mathfrak{g}^*$  (cf. Subsection 4.4), one may form another phase space  $M//G = \mu^{-1}(0)/G$ .<sup>179</sup> Physically, in the case where  $G$  is a gauge group and  $M$  is the unconstrained phase space,  $\mu^{-1}(0)$  is the constraint hypersurface (i.e. the

<sup>176</sup>Using the formalism explained in footnote 167, we replace the 1-form  $A = -\frac{i}{\hbar} \sum_k p_k dq^k$  defining the connection  $\nabla = d + A$  by the gauge-equivalent form  $A = \frac{i}{2\hbar} (\sum_k q^k dp_k - \sum_k p_k dq^k) = -\frac{i}{\hbar} \sum_k p_k dq^k + \frac{i}{2\hbar} d(\sum_k p_k q^k)$ , which has the same curvature. In terms of this new  $A$ , which in complex coordinates reads  $A = \sum_k (z_k d\bar{z}_k - \bar{z}_k dz_k)/4\hbar$ , eq. (47) is just  $\nabla_{\partial/\partial \bar{z}} \Phi = 0$ . This is an example of the so-called holomorphic polarization in the formalism of geometric quantization.

<sup>177</sup>The collection of all holomorphic functions on  $\mathbb{C}$  satisfying (49) is a Hilbert space with respect to the inner product  $(f, g) = (2\pi\hbar i)^{-1} \int_{\mathbb{C}} dz d\bar{z} \exp(-|z|^2/2\hbar) \overline{f(z)} g(z)$ , called the *Bargmann–Fock space*  $\mathcal{H}_{BF}$ . This space may be embedded in  $L^2(\mathbb{C})$  by  $f(z) \mapsto \exp(-|z|^2/2\hbar) f(z)$ , and the image of this embedding is of course just  $pL^2(\mathbb{C})$ .

<sup>178</sup>See [Gotay *et al.*, 1978; Binz *et al.*, 1988; Marsden, 1992; Marsden and Ratiu, 1994; Landsman, 1998; Butterfield, 2005], and [Belot, 2005].

<sup>179</sup>Technically,  $M$  has to be a symplectic manifold, and if  $G$  acts properly and freely on  $\mu^{-1}(0)$ , then  $M//G$  is again a symplectic manifold.

subspace of  $M$  on which the constraints defined by the gauge symmetry hold), and  $M//G$  is the true phase space of the system that only contains physical degrees of freedom.

Unfortunately, the correct way of dealing with constrained quantum systems remains a source of speculation and controversy:<sup>180</sup> practically all rigorous results on quantization (like the ones discussed in the preceding subsections) concern unconstrained systems. Accordingly, one would like to quantize a constrained system by reducing the problem to the unconstrained case. This could be done provided the following scenario applies. One first quantizes the unconstrained phase space  $M$  (supposedly the easiest part of the problem), and subsequently imposes a quantum version of symplectic reduction. Finally, one proves by abstract means that the quantum theory thus constructed is equal to the theory defined by first reducing at the classical level and then quantizing the constrained classical phase space (usually an impossible task to perform in practice).

Tragically, sufficiently powerful theorems stating that “quantization commutes with reduction” in this sense remain elusive.<sup>181</sup> So far, this has blocked, for example, a rigorous quantization of Yang–Mills theory in dimension 4; this is one of the Millennium Problems of the Clay Mathematical Institute, rewarded with 1 Million dollars.<sup>182</sup>

On a more spiritual note, the mathematician E. Nelson famously said that ‘First quantization is a mystery, but second quantization is a functor.’ The functoriality of ‘second’ quantization (a construction involving Fock spaces, see [Reed and Simon, 1975] being an almost trivial matter, the deep mathematical and conceptual problem lies in the possible functoriality of ‘first’ quantization, which simply means quantization in the sense we have been discussing so far. This was initially taken to mean that canonical transformations  $\alpha$  of the phase space  $M$  should be ‘quantized’ by unitary operators  $U(\alpha)$  on  $\mathcal{H}(M)$ , in such a way  $U(\alpha)\mathcal{Q}_\hbar(f)U(\alpha)^{-1} = \mathcal{Q}(L_\alpha f)$  (cf. (10)). This is possible only in special circumstances, e.g., when  $M = \mathbb{R}^{2n}$  and  $\alpha$  is a linear symplectic map, and more generally when  $M = G/H$  is homogeneous and  $\alpha \in G$  (see the end of Subsection 4.2).<sup>183</sup> Consequently, the functoriality of quantization is widely taken to be a dead end.<sup>184</sup>

However, all no-go theorems establishing this conclusion start from wrong and

<sup>180</sup>Cf. [Dirac, 1964; Sundermeyer, 1982; Gotay, 1986; Duval *et al.*, 1991; Govaerts, 1991; Henneaux and Teitelboim, 1992], and [Landsman, 1998] for various perspectives on the quantization of constrained systems.

<sup>181</sup>The so-called Guillemin–Sternberg conjecture [Guillemin and Sternberg, 1982] — now a theorem [Meinrenken, 1998; Meinrenken and Sjamaar, 1999] — merely deals with the case of Marsden–Weinstein reduction where  $G$  and  $M$  are compact. Mathematically impressive as the “quantization commutes with reduction” theorem already is here, it is a far call from gauge theories, where the groups and spaces are not only noncompact but even infinite-dimensional.

<sup>182</sup>See <http://www.claymath.org/millennium/>

<sup>183</sup>Canonical transformations *can* be quantized in approximate sense that becomes precise as  $\hbar \rightarrow 0$  by means of so-called Fourier integral operators; see [Hörmander, 1971; 1985b] and [Duistermaat, 1996].

<sup>184</sup>See [Groenewold, 1946; van Hove, 1951; Gotay *et al.*, 1996], and [Gotay, 1999].

naive categories, both on the classical and on the quantum side.<sup>185</sup> It appears very likely that one may indeed make quantization functorial by a more sophisticated choice of categories, with the additional bonus that deformation quantization and geometric quantization become unified: the former is the object part of the quantization functor, whereas the latter (suitably reinterpreted) is the arrow part. Amazingly, on this formulation the statement that ‘quantization commutes with reduction’ becomes a special case of the functoriality of quantization [Landsman, 2002; 2005].

To explain the main idea, we return to the geometric quantization of  $M = \mathbb{R}^2 \cong \mathbb{C}$  explained in the preceding subsection. The identification of  $pL^2(\mathbb{C})$ <sup>186</sup> as the correct Hilbert space of the problem may be understood in a completely different way, which paves the way for the powerful reformulation of the geometric quantization program that will eventually define the quantization functor. Namely,  $\mathbb{C}$  supports a certain linear first-order differential operator  $\mathcal{D}$  that is entirely defined by its geometry as a phase space, called the *Dirac operator*.<sup>187</sup> This operator is given by<sup>188</sup>

$$(50) \quad \mathcal{D} = 2 \begin{pmatrix} 0 & -\frac{\partial}{\partial z} + \frac{\bar{z}}{4\hbar} \\ \frac{\partial}{\partial \bar{z}} + \frac{z}{4\hbar} & 0 \end{pmatrix},$$

acting on  $L^2(\mathbb{C}) \otimes \mathbb{C}^2$  (as a suitably defined unbounded operator). This operator has the generic form

$$\mathcal{D} = \begin{pmatrix} 0 & \mathcal{D}_- \\ \mathcal{D}_+ & 0 \end{pmatrix}.$$

The *index* of such an operator is given by

$$(51) \quad \text{index}(\mathcal{D}) = [\ker(\mathcal{D}_+)] - [\ker(\mathcal{D}_-)],$$

where  $[\ker(\mathcal{D}_\pm)]$  stand for the (unitary) isomorphism class of  $\ker(\mathcal{D}_\pm)$  *seen as a representation space of a suitable algebra of operators*.<sup>189</sup> In the case at hand,

<sup>185</sup>Typically, one takes the classical category to consist of symplectic manifolds as objects and symplectomorphisms as arrows, and the quantum category to have  $C^*$ -algebras as objects and automorphisms as arrows.

<sup>186</sup>Or the Bargmann–Fock space  $\mathcal{H}_{BF}$ , see footnote 177.

<sup>187</sup>Specifically, this is the so-called  $\text{Spin}^c$  Dirac operator defined by the complex structure of  $\mathbb{C}$ , *coupled to the prequantization line bundle*. See [Guillemin *et al.*, 2002].

<sup>188</sup>Relative to the Dirac matrices  $\gamma^1 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$  and  $\gamma^2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ .

<sup>189</sup>The left-hand side of (51) should really be written as  $\text{index}(\mathcal{D}_+)$ , since  $\text{coker}(\mathcal{D}_+) = \ker(\mathcal{D}_+^*)$  and  $\mathcal{D}_+^* = \mathcal{D}_-$ , but since the index is naturally associated to  $\mathcal{D}$  as a whole, we abuse notation in writing  $\text{index}(\mathcal{D})$  for  $\text{index}(\mathcal{D}_+)$ . The usual index of a linear map  $L : V \rightarrow W$  between finite-dimensional vector spaces is defined as  $\text{index}(L) = \dim(\ker(L)) - \dim(\text{coker}(L))$ , where  $\text{coker}(L) = W/\text{ran}(L)$ . Elementary linear algebra yields  $\text{index}(L) = \dim(V) - \dim(W)$ . This is surprising because it is independent of  $L$ , whereas  $\dim(\ker(L))$  and  $\dim(\text{coker}(L))$  quite sensitively depend on it. For, example, take  $V = W$  and  $L = \varepsilon \cdot 1$ . If  $\varepsilon \neq 0$  then  $\dim(\ker(\varepsilon \cdot 1)) = \dim(\text{coker}(\varepsilon \cdot 1)) = 0$ , whereas for  $\varepsilon = 0$  one has  $\dim(\ker(0)) = \dim(\text{coker}(0)) = \dim(V)$ ! Similarly, the usual definition of geometric quantization through (47) etc. is unstable against perturbations of the underlying symplectic structure, whereas the refined definition through (51) is not. To

one has  $\ker(\mathcal{D}_+) = pL^2(\mathbb{C})$  (cf. (47) etc.) and  $\ker(\mathcal{D}_-) = 0$ ,<sup>190</sup> where we regard  $\ker(\mathcal{D}_+)$  as a representation space of the Heisenberg group  $H_1$ . Consequently, the geometric quantization of the phase space  $\mathbb{C}$  is given *modulo unitary equivalence* by  $\text{index}(\mathcal{D})$ , seen as a “formal difference” of representation spaces of  $H_1$ .

This procedure may be generalized to arbitrary phase spaces  $M$ , where  $\mathcal{D}$  is a certain operator naturally defined by the phase space geometry of  $M$  and the demands of quantization.<sup>191</sup> This has turned out to be the most promising formulation of geometric quantization — at some cost.<sup>192</sup> For the original goal of quantizing a phase space by a Hilbert space has now been replaced by a much more abstract procedure, in which the result of quantization is a formal difference of certain isomorphism classes of representation spaces of the quantum algebra of observables. To illustrate the degree of abstraction involved here, suppose we ignore the action of the observables (such as position and momentum in the example just considered). In that case the isomorphism class  $[\mathcal{H}]$  of a Hilbert space  $\mathcal{H}$  is entirely characterized by its dimension  $\dim(\mathcal{H})$ , so that (in case that  $\ker(\mathcal{D}_-) \neq 0$ ) quantization (in the guise of  $\text{index}(\mathcal{D})$ ) can even be a negative number! Have we gone mad?

Not quite. The above picture of geometric quantization is indeed quite irrelevant to physics, *unless it is supplemented by deformation quantization*. It is convenient to work at some fixed value of  $\hbar$  in this context, so that deformation quantization merely associates some  $C^*$ -algebra  $\mathcal{A}(P)$  to a given phase space  $P$ .<sup>193</sup> Looking for a categorical interpretation of quantization, it is therefore natural to assume that the objects of the classical category  $\mathfrak{C}$  are phase spaces  $P$ ,<sup>194</sup> whereas the

pass to the latter from the above notion of an index, we first write  $\text{index}(L) = [\ker(L)] - [\text{coker}(L)]$ , where  $[X]$  is the isomorphism class of a linear space  $X$  as a  $\mathbb{C}$ -module. This expression is an element of  $K_0(\mathbb{C})$ , and we recover the earlier index through the realization that the class  $[X]$  is entirely determined by  $\dim(X)$ , along with and the corresponding isomorphism  $K_0(\mathbb{C}) \cong \mathbb{Z}$ . When a more complicated finite-dimensional  $C^*$ -algebra  $\mathcal{A}$  acts on  $V$  and  $W$  with the property that  $\ker(L)$  and  $\text{coker}(L)$  are stable under the  $\mathcal{A}$ -action, one may define  $[\ker(L)] - [\text{coker}(L)]$  and hence  $\text{index}(L)$  as an element of the so-called  $C^*$ -algebraic K-theory group  $K_0(\mathcal{A})$ . Under certain technical conditions, this notion of an index may be generalized to infinite-dimensional Hilbert spaces and  $C^*$ -algebras; see [Baum *et al.*, 1994] and [Blackadar, 1998]. The K-theoretic index is best understood when  $\mathcal{A} = C^*(G)$  is the group  $C^*$ -algebra of some locally compact group  $G$ . In the example  $M = \mathbb{R}^2$  one might take  $G$  to be the Heisenberg group  $H_1$ , so that  $\text{index}(\mathcal{D}) \in K_0(C^*(H_1))$ . See [Elliott *et al.*, 1993] for a description of this  $K_0$ -group.

<sup>190</sup>Since  $(-\frac{\partial}{\partial z} + \frac{\bar{z}}{4\hbar})\Phi = 0$  implies  $\Phi(z, \bar{z}) = \exp(|z|^2/4\hbar)f(\bar{z})$ , which lies in  $L^2(\mathbb{C})$  iff  $f = 0$ .

<sup>191</sup>Any symplectic manifold carries an almost complex structure compatible with the symplectic form, leading to a  $\text{Spin}^c$  Dirac operator as described in footnote 187. See, again, [Guillemin *et al.*, 2002]. If  $M = G/H$ , or, more generally, if  $M$  carries a canonical action of a Lie group  $G$  with compact quotient  $M/G$ , then  $\text{index}(\mathcal{D})$  defines an element of  $K_0(C^*(G))$ . See footnote 189. In complete generality,  $\text{index}(\mathcal{D})$  ought to be an element of  $K_0(\mathcal{A})$ , where  $\mathcal{A}$  is the  $C^*$ -algebra of observables of the quantum system.

<sup>192</sup>On the benefit side, the invariance of the index under continuous deformations of  $\mathcal{D}$  seems to obviate the ambiguity of traditional quantization procedures with respect to different ‘operator orderings’ not prescribed by the classical theory.

<sup>193</sup>Here  $P$  is not necessarily symplectic; it may be a Poisson manifold, and to keep Poisson and symplectic manifolds apart we denote the former by  $P$  from now on, preserving the notation  $M$  for the latter.

<sup>194</sup>Strictly speaking, to be an object in this category a Poisson manifold  $P$  must be *integrable*;

objects of the quantum category  $\mathfrak{Q}$  are  $C^*$ -algebras.<sup>195</sup> The object part of the hypothetical quantization functor is to be deformation quantization, symbolically written as  $P \mapsto \mathcal{Q}(P)$ .

Everything then fits together if geometric quantization is reinterpreted as the arrow part of the conjectural quantization functor. To accomplish this, the arrows in the classical category  $\mathfrak{C}$  should not be taken to be maps between phase spaces, but *symplectic bimodules*  $P_1 \leftarrow M \rightarrow P_2$ .<sup>196</sup> More precisely, the arrows in  $\mathfrak{C}$  are suitable isomorphism classes of such bimodules.<sup>197</sup> Similarly, the arrows in the quantum category  $\mathfrak{Q}$  are not morphisms of  $C^*$ -algebras, as might naively be expected, but certain isomorphism classes of bimodules for  $C^*$ -algebras, equipped with the additional structure of a generalized Dirac operator.<sup>198</sup>

Having already defined the object part of the quantization map  $\mathcal{Q} : \mathfrak{C} \rightarrow \mathfrak{Q}$  as deformation quantization, we now propose that the arrow part is geometric quantization, in the sense of a suitable generalization of (51); see [Landsman, 2005] for details. We then conjecture that  $\mathcal{Q}$  is a functor; in the cases where this can and has been checked, the functoriality of  $\mathcal{Q}$  is precisely the statement that quantization commutes with reduction.<sup>199</sup>

Thus Heisenberg's idea of *Umdeutung* finds its ultimate realization in the quantization functor.

## 5 THE LIMIT $\hbar \rightarrow 0$

It was recognized at an early stage that the limit  $\hbar \rightarrow 0$  of Planck's constant going to zero should play a role in the explanation of the classical world from quantum theory. Strictly speaking,  $\hbar$  is a dimensionful *constant*, but in practice one studies the semiclassical regime of a given quantum theory by forming a dimensionless combination of  $\hbar$  and other parameters; this combination then re-enters the theory as if it were a dimensionless version of  $\hbar$  that can indeed be varied. The oldest example is Planck's radiation formula (1), with temperature  $T$  as the pertinent

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see [Landsman, 2001].

<sup>195</sup>For technical reasons involving  $K$ -theory these have to be separable.

<sup>196</sup>Here  $M$  is a symplectic manifold and  $P_1$  and  $P_2$  are integrable Poisson manifolds; the map  $M \rightarrow P_2$  is anti-Poisson, whereas the map  $P_1 \leftarrow M$  is Poisson. Such bimodules (often called *dual pairs*) were introduced by Karasev [1989] and Weinstein [1983]. In order to occur as arrows in  $\mathfrak{C}$ , symplectic bimodules have to satisfy a number of regularity conditions [Landsman, 2001].

<sup>197</sup>This is necessary in order to make arrow composition associative; this is given by a generalization of the symplectic reduction procedure.

<sup>198</sup>The category  $\mathfrak{Q}$  is nothing but the category  $KK$  introduced by Kasparov, whose objects are separable  $C^*$ -algebras, and whose arrows are the so-called Kasparov group  $KK(A, B)$ , composed with Kasparov's product  $KK(A, B) \times KK(B, C) \rightarrow KK(A, C)$ . See [Higson, 1990] and [Blackadar, 1998].

<sup>199</sup>A canonical  $G$ -action on a symplectic manifold  $M$  with momentum map  $\mu : M \rightarrow \mathfrak{g}^*$  gives rise to a dual pair  $pt \leftarrow M \rightarrow \mathfrak{g}^*$ , which in  $\mathfrak{C}$  is interpreted as an arrow from the space  $pt$  with one point to  $\mathfrak{g}^*$ . The composition of this arrow with the arrow  $\mathfrak{g}^* \leftarrow 0 \rightarrow pt$  from  $\mathfrak{g}^*$  to  $pt$  is  $pt \leftarrow M//G \rightarrow pt$ . If  $G$  is connected, functoriality of quantization on these two pairs is equivalent to the Guillemin–Sternberg conjecture (cf. footnote 181); see [Landsman, 2005].

variable. Indeed, the observation of Einstein [1905] and Planck [1906] that in the limit  $\hbar\nu/kT \rightarrow 0$  this formula converges to the classical equipartition law  $E_\nu/N_\nu = kT$  may well be the first use of the  $\hbar \rightarrow 0$  limit of quantum theory.<sup>200</sup>

Another example is the Schrödinger equation (3) with Hamiltonian  $H = -\frac{\hbar^2}{2m}\Delta_x + V(x)$ , where  $m$  is the mass of the pertinent particle. Here one may pass to dimensionless parameters by introducing an energy scale  $\epsilon$  typical of  $H$ , like  $\epsilon = \sup_x |V(x)|$ , as well as a typical length scale  $\lambda$ , such as  $\lambda = \epsilon/\sup_x |\nabla V(x)|$  (if these quantities are finite). In terms of the dimensionless variable  $\tilde{x} = x/\lambda$ , the rescaled Hamiltonian  $\tilde{H} = H/\epsilon$  is then dimensionless and equal to  $\tilde{H} = -\tilde{\hbar}^2\Delta_{\tilde{x}} + \tilde{V}(\tilde{x})$ , where  $\tilde{\hbar} = \hbar/\lambda\sqrt{2m\epsilon}$  and  $\tilde{V}(\tilde{x}) = V(\lambda\tilde{x})/\epsilon$ . Here  $\tilde{\hbar}$  is dimensionless, and one might study the regime where it is small [Gustafson and Sigal, 2003]. Our last example will occur in the theory of large quantum systems, treated in the next Section. In what follows, whenever it is considered variable  $\hbar$  will denote such a dimensionless version of Planck's constant.

Although, as we will argue, the limit  $\hbar \rightarrow 0$  cannot by itself explain the classical world, it does give rise to a number of truly pleasing mathematical results. These, in turn, render almost inescapable the conclusion that the limit in question is indeed a relevant one for the recovery of classical physics from quantum theory. Thus the present section is meant to be a catalogue of those pleasantries that might be of direct interest to researchers in the foundations of quantum theory.

There is another, more technical use of the  $\hbar \rightarrow 0$  limit, which is to perform computations in quantum mechanics by approximating the time-evolution of states and observables in terms of associated classical objects. This endeavour is known as *semiclassical analysis*. Mathematically, this use of the  $\hbar \rightarrow 0$  limit is closely related to the goal of recovering classical mechanics from quantum mechanics, but conceptually the matter is quite different. We will attempt to bring the pertinent differences out in what follows.

### 5.1 Coherent states revisited

As Schrödinger [1926b] foresaw, coherent states play an important role in the limit  $\hbar \rightarrow 0$ . We recall from Subsection 4.2 that *for some fixed value  $\hbar$  of Planck's constant* coherent states in a Hilbert space  $\mathcal{H}$  for a phase space  $M$  are defined by an injection  $M \hookrightarrow \mathcal{H}$ ,  $z \mapsto \Psi_z^\hbar$ , such that (16) and (17) hold. In what follows, we shall say that  $\Psi_z^\hbar$  is *centered at  $z \in M$* , a terminology justified by the key example (20).

To be relevant to the classical limit, coherent states must satisfy an additional property concerning their dependence on  $\hbar$ , which also largely clarifies their nature [Landsman, 1998]. Namely, we require that for each  $f \in C_c(M)$  and each  $z \in M$  the following function from the set  $I$  in which  $\hbar$  takes values (i.e. usually  $I = [0, 1]$ ,

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<sup>200</sup>Here Einstein [1905] put  $\hbar\nu/kT \rightarrow 0$  by letting  $\nu \rightarrow 0$  at fixed  $T$  and  $\hbar$ , whereas Planck [1906] took  $T \rightarrow \infty$  at fixed  $\nu$  and  $\hbar$ .



but in any case containing zero as an accumulation point) to  $\mathbb{C}$  is continuous:

- (1)  $\hbar \mapsto c_{\hbar} \int_M d\mu_L(w) |(\Psi_w^{\hbar}, \Psi_z^{\hbar})|^2 f(w) \quad (\hbar > 0);$
- (2)  $0 \mapsto f(z).$

In view of (19), the right-hand side of (2) is the same as  $(\Psi_z^{\hbar}, \mathcal{Q}_{\hbar}^B(f)\Psi_z^{\hbar})$ . In particular, this continuity condition implies

$$(3) \quad \lim_{\hbar \rightarrow 0} (\Psi_z^{\hbar}, \mathcal{Q}_{\hbar}^B(f)\Psi_z^{\hbar}) = f(z).$$

This means that the classical limit of the quantum-mechanical expectation value of the phase space quantization (19) of the classical observable  $f$  in a coherent state centered at  $z \in M$  is precisely the classical expectation value of  $f$  in the state  $z$ . This interpretation rests on the identification of classical states with probability measures on phase space  $M$ , under which points of  $M$  in the guise of Dirac measures (i.e. delta functions) are pure states. Furthermore, it can be shown (cf. [Landsman, 1998]) that the continuity of all functions (1) - (2) implies the property

$$(4) \quad \lim_{\hbar \rightarrow 0} |(\Psi_w^{\hbar}, \Psi_z^{\hbar})|^2 = \delta_{wz},$$

where  $\delta_{wz}$  is the ordinary Kronecker delta (i.e.  $\delta_{wz} = 0$  whenever  $w \neq z$  and  $\delta_{zz} = 1$  for all  $z \in M$ ). This has a natural physical interpretation as well: the classical limit of the quantum-mechanical transition probability between two coherent states centered at  $w, z \in M$  is equal to the classical (and trivial) transition probability between  $w$  and  $z$ . In other words, when  $\hbar$  becomes small, coherent states at different values of  $w$  and  $z$  become increasingly orthogonal to each other.<sup>201</sup> This has the interesting consequence that

$$(5) \quad \lim_{\hbar \rightarrow 0} (\Psi_w^{\hbar}, \mathcal{Q}_{\hbar}^B(f)\Psi_z^{\hbar}) = 0 \quad (w \neq z).$$

for all  $f \in C_c(M)$ . In particular, the following phenomenon of the Schrödinger cat type occurs in the classical limit: if  $w \neq z$  and one has continuous functions  $\hbar \mapsto c_w^{\hbar} \in \mathbb{C}$  and  $\hbar \mapsto c_z^{\hbar} \in \mathbb{C}$  on  $\hbar \in [0, 1]$  such that

$$(6) \quad \Psi_{w,z}^{\hbar} = c_w^{\hbar} \Psi_w^{\hbar} + c_z^{\hbar} \Psi_z^{\hbar}$$

is a unit vector for  $\hbar \geq 0$  and also  $|c_w^0|^2 + |c_z^0|^2 = 1$ , then

$$(7) \quad \lim_{\hbar \rightarrow 0} (\Psi_{w,z}^{\hbar}, \mathcal{Q}_{\hbar}^B(f)\Psi_{w,z}^{\hbar}) = |c_w^0|^2 f(w) + |c_z^0|^2 f(z).$$

Hence the family of (typically) pure states  $\psi_{w,z}^{\hbar}$  (on the  $C^*$ -algebras  $\mathcal{A}_{\hbar}$  in which the map  $\mathcal{Q}_{\hbar}^B$  takes values)<sup>202</sup> defined by the vectors  $\Psi_{w,z}^{\hbar}$  in some sense converges

<sup>201</sup>See [Mielnik, 1968; Cantoni, 1975; Beltrametti and Cassinelli, 1984; Landsman, 1998], and Subsection 6.3 below for the general meaning of the concept of a transition probability.

<sup>202</sup>For example, for  $M = \mathbb{R}^{2n}$  each  $\mathcal{A}_{\hbar}$  is equal to the  $C^*$ -algebra of compact operators on  $L^2(\mathbb{R}^n)$ , on which each vector state is certainly pure.

to the mixed state on  $C_0(M)$  defined by the right-hand side of (7). This is made precise at the end of this subsection.

It goes without saying that Schrödinger’s coherent states (20) satisfy our axioms; one may also verify (4) immediately from (21). Consequently, by (32) one has the same property (3) for Weyl quantization (as long as  $f \in \mathcal{S}(\mathbb{R}^{2n})$ ),<sup>203</sup> that is,

$$(8) \quad \lim_{\hbar \rightarrow 0} (\Psi_z^\hbar, \mathcal{Q}_\hbar^W(f), \Psi_z^\hbar) = f(z).$$

Similarly, (5) holds for  $\mathcal{Q}_\hbar^W$  as well.

In addition, many constructions referred to as coherent states in the literature (cf. the references in footnote 129) satisfy (16), (17), and (4); see [Landsman, 1998].<sup>204</sup> The general picture that emerges is that a coherent state centered at  $z \in M$  is the *Umdeutung* of  $z$  (seen as a classical pure state, as explained above) as a quantum-mechanical pure state.<sup>205</sup>

Despite their wide applicability (and some would say beauty), one has to look beyond coherent states for a complete picture of the  $\hbar \rightarrow 0$  limit of quantum mechanics. The appropriate generalization is the concept of a *continuous field of states*.<sup>206</sup> This is defined relative to a given deformation quantization of a phase space  $M$ ; cf. Subsection 4.3. If one now has a state  $\omega_\hbar$  on  $\mathcal{A}_\hbar$  for each  $\hbar \in [0, 1]$  (or, more generally, for a discrete subset of  $[0, 1]$  containing 0 as an accumulation point), one may call the ensuing family of states a *continuous field* whenever the function  $\hbar \mapsto \omega_\hbar(\mathcal{Q}_\hbar(f))$  is continuous on  $[0, 1]$  for each  $f \in C_c^\infty(M)$ ; this notion is actually intrinsically defined by the continuous field of  $C^*$ -algebras, and is therefore independent of the quantization maps  $\mathcal{Q}_\hbar$ . In particular, one has

$$(9) \quad \lim_{\hbar \rightarrow 0} \omega_\hbar(\mathcal{Q}_\hbar(f)) = \omega_0(f).$$

Eq. (3) (or (8)) shows that coherent states are indeed examples of continuous fields of states, with the additional property that each  $\omega_\hbar$  is pure. As an example where all states  $\omega_\hbar$  are mixed, we mention the convergence of quantum-mechanical

<sup>203</sup>Here  $\mathcal{S}(\mathbb{R}^{2n})$  is the usual Schwartz space of smooth test functions with rapid decay at infinity.

<sup>204</sup>For example, coherent states of the type introduced by Perelomov [1986] fit into our setting as follows [Simon, 1980]. Let  $G$  be a compact connected Lie group, and  $\mathcal{O}_\lambda$  an integral coadjoint orbit, corresponding to a highest weight  $\lambda$ . (One may think here of  $G = SU(2)$  and  $\lambda = 0, 1/2, 1, \dots$ ) Note that  $\mathcal{O}_\lambda \cong G/T$ , where  $T$  is the maximal torus in  $G$  with respect to which weights are defined. Let  $\mathcal{H}_\lambda^{\text{hw}}$  be the carrier space of the irreducible representation  $U_\lambda(G)$  with highest weight  $\lambda$ , containing the highest weight vector  $\Omega_\lambda$ . (For  $G = SU(2)$  one has  $\mathcal{H}_j^{\text{hw}} = \mathbb{C}^{2j+1}$ , the well-known Hilbert space of spin  $j$ , in which  $\Omega_j$  is the vector with spin  $j$  in the  $z$ -direction.) For  $\hbar = 1/k$ ,  $k \in \mathbb{N}$ , define  $\mathcal{H}_\hbar := \mathcal{H}_{\lambda/\hbar}^{\text{hw}}$ . Choosing a section  $\sigma : \mathcal{O}_\lambda \rightarrow G$  of the projection  $G \rightarrow G/T$ , one then obtains coherent states  $x \mapsto U_{\lambda/\hbar}(\sigma(x))\Omega_{\lambda/\hbar}$  with respect to the Liouville measure on  $\mathcal{O}_\lambda$  and  $c_\hbar = \dim(\mathcal{H}_{\lambda/\hbar}^{\text{hw}})$ . These states are obviously not defined for all values of  $\hbar$  in  $(0, 1]$ , but only for the discrete set  $1/\mathbb{N}$ .

<sup>205</sup>This idea is also confirmed by the fact that at least Schrödinger’s coherent states are states of minimal uncertainty; cf. the references in footnote 129.

<sup>206</sup>The use of this concept in various mathematical approaches to quantization is basically folklore. For the  $C^*$ -algebraic setting see [Emch, 1984; Rieffel, 1989b; Werner, 1995; Blanchard, 1996; Landsman, 1998], and [Nagy, 2000].

partition functions to their classical counterparts in statistical mechanics along these lines; see [Lieb, 1973; Simon, 1980; Duffield, 1990], and [Nourrigat and Royer, 2004]. Finally, one encounters the phenomenon that pure quantum states may coverge to mixed classical ones. The first example of this has just been exhibited in (7); other cases in point are energy eigenstates and WKB states (see Subsections 5.4, 5.5, and 5.6 below).

## 5.2 Convergence of quantum dynamics to classical motion

Nonrelativistic quantum mechanics is based on the Schrödinger equation (3), which more generally reads

$$(10) \quad H\Psi(t) = i\hbar \frac{\partial \Psi}{\partial t}.$$

The formal solution with initial value  $\Psi(0) = \Psi$  is

$$(11) \quad \Psi(t) = e^{-\frac{it}{\hbar}H}\Psi.$$

Here we have assumed that  $H$  is a given self-adjoint operator on the Hilbert space  $\mathcal{H}$  of the system, so that this solution indeed exists and evolves unitarily by Stone's theorem; cf. [Reed and Simon, 1972] and [Simon, 1976]. Equivalently, one may transfer the time-evolution from states (Schrödinger picture) to operators (Heisenberg picture) by putting

$$(12) \quad A(t) = e^{\frac{it}{\hbar}H} A e^{-\frac{it}{\hbar}H}.$$

We here restrict ourselves to particle motion in  $\mathbb{R}^n$ , so that  $\mathcal{H} = L^2(\mathbb{R}^n)$ .<sup>207</sup> In that case,  $H$  is typically given by a formal expression like (3) (on some specific domain).<sup>208</sup> Now, the first thing that comes to mind is *Ehrenfest's Theorem* [1927], which states that for any (unit) vector  $\Psi \in L^2(\mathbb{R}^n)$  in the domain of  $\mathcal{Q}_\hbar(q^j) = x^j$  and  $\partial V(x)/\partial x^j$  one has

$$(13) \quad m \frac{d^2}{dt^2} \langle x^j \rangle(t) = - \left\langle \frac{\partial V(x)}{\partial x^j} \right\rangle(t),$$

with the notation

$$(14) \quad \begin{aligned} \langle x^j \rangle(t) &= (\Psi(t), x^j \Psi(t)); \\ \left\langle \frac{\partial V(x)}{\partial x^j} \right\rangle(t) &= \left( \Psi(t), \frac{\partial V(x)}{\partial x^j} \Psi(t) \right). \end{aligned}$$

This looks like Newton's second law for the expectation value of  $x$  in the state  $\psi$ , with the tiny but crucial difference that Newton would have liked to see  $(\partial V/\partial x^j)(\langle x \rangle(t))$  on the right-hand side of (13). Furthermore, even apart from

<sup>207</sup>See [Hunziker and Sigal, 2000] for a recent survey of  $N$ -body Schrödinger operators.

<sup>208</sup>One then has to prove self-adjointness (or the lack of it) on a larger domain on which the operator is closed; see the literature cited in footnote 42.

this point Ehrenfest's Theorem by no means suffices to have classical behaviour, since it gives no guarantee whatsoever that  $\langle x \rangle(t)$  behaves like a point particle. Much of what follows can be seen as an attempt to sharpen Ehrenfest's Theorem to the effect that it *does* indeed yield appropriate classical equations of motion for the expectation values of suitable operators.

We assume that the quantum Hamiltonian has the more general form

$$(15) \quad H = h(\mathcal{Q}_{\hbar}(p_j), \mathcal{Q}_{\hbar}(q^j)),$$

where  $h$  is the classical Hamiltonian (i.e. a function defined on classical phase space  $\mathbb{R}^{2n}$ ) and  $\mathcal{Q}_{\hbar}(p_j)$  and  $\mathcal{Q}_{\hbar}(q^j)$  are the operators given in (2). Whenever this expression is ambiguous (as in cases like  $h(p, q) = pq$ ), one has to assume a specific quantization prescription such as Weyl quantization  $\mathcal{Q}_{\hbar}^W$  (cf. (29)), so that formally one has

$$(16) \quad H = \mathcal{Q}_{\hbar}^W(h).$$

In fact, in the literature to be cited an even larger class of quantum Hamiltonians is treated by the methods explained here. The quantum Hamiltonian  $H$  carries an explicit (and rather singular)  $\hbar$ -dependence, and for  $\hbar \rightarrow 0$  one then expects (11) or (12) to be related in one way or another to the flow of the classical Hamiltonian  $h$ . This relationship was already foreseen by Schrödinger (1926a), and was formalized almost immediately after the birth of quantum mechanics by the well-known WKB approximation (cf. [Landau and Lifshitz, 1977] and Subsection 5.5 below). A mathematically rigorous understanding of this and analogous approximation methods only emerged much later, when a technique called *microlocal analysis* was adapted from its original setting of partial differential equations [Hörmander, 1965; Kohn and Nirenberg, 1965; Duistermaat, 1974; 1996; Guillemin and Sternberg, 1977; Howe, 1980; Hörmander, 1979; 1985a; 1985b; Grigis and Sjöstrand, 1994] to the study of the  $\hbar \rightarrow 0$  limit of quantum mechanics. This adaptation (often called *semiclassical analysis*) and its results have now been explained in various reviews written by the main players, notably [Robert, 1987; 1998; Helffer, 1988; Paul and Uribe, 1995; Colin de Verdière, 1998; Ivrii, 1998; Dimassi and Sjöstrand, 1999], and [Martinez, 2002] (see also the papers in [Robert, 1992]). More specific references will be given below.<sup>209</sup>

As mentioned before, the relationship between  $H$  and  $h$  provided by semiclassical analysis is double-edged. On the one hand, one obtains approximate solutions of (11) or (12), or approximate energy eigenvalues and energy eigenfunctions (sometimes called quasi-modes) for small values of  $\hbar$  in terms of classical data. This is how the results are usually presented; one computes specific properties of quantum theory in a certain regime in terms of an underlying classical theory. On the other hand, however, with some effort the very same results can often be reinterpreted as a partial explanation of the emergence of classical dynamics from

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<sup>209</sup>For the heuristic theory of semiclassical asymptotics [Landau and Lifshitz, 1977] is a goldmine.

quantum mechanics. It is the latter aspect of semiclassical analysis, somewhat understated in the literature, that is of interest to us. In this and the next three subsections we restrict ourselves to the simplest type of results, which nonetheless provide a good flavour of what can be achieved and understood by these means. By the same token, we just work with the usual flat phase space  $M = \mathbb{R}^{2n}$  as before.

The simplest of all results relating classical and quantum dynamics is this:<sup>210</sup>

*If the classical Hamiltonian  $h(p, q)$  is at most quadratic in  $p$  and  $q$ , and the Hamiltonian in (12) is given by (16), then*

$$(17) \quad \mathcal{Q}_\hbar^W(f)(t) = \mathcal{Q}_\hbar^W(f_t).$$

Here  $f_t$  is the solution of the classical equation of motion  $df_t/dt = \{h, f_t\}$ ; equivalently, one may write

$$(18) \quad f_t(p, q) = f(p(t), q(t)),$$

where  $t \mapsto (p(t), q(t))$  is the classical Hamiltonian flow of  $h$  with initial condition  $(p(0), q(0)) = (p, q)$ . This holds for all decent  $f$ , e.g.,  $f \in \mathcal{S}(\mathbb{R}^{2n})$ .

This result explains quantum in terms of classical, but the converse may be achieved by combining (17) with (9). This yields

$$(19) \quad \lim_{\hbar \rightarrow 0} \omega_\hbar(\mathcal{Q}_\hbar(f)(t)) = \omega_0(f_t)$$

for any continuous field of states  $(\omega_\hbar)$ . In particular, for Schrödinger's coherent states (20) one obtains

$$(20) \quad \lim_{\hbar \rightarrow 0} \left( \Psi_{(p,q)}^\hbar, \mathcal{Q}_\hbar(f)(t) \Psi_{(p,q)}^\hbar \right) = f_t(p, q).$$

Now, whereas (17) merely reflects the good symmetry properties of Weyl quantization,<sup>211</sup> (and is false for  $\mathcal{Q}_\hbar^B$ ), eq. (20) is actually valid for a large class of realistic Hamiltonians and for any deformation quantization map  $\mathcal{Q}_\hbar$  that is asymptotically equal to  $\mathcal{Q}_\hbar^W$  (cf. (32)). A result of this type was first established by Hepp [1974]; further work in this direction includes [Yajima, 1979; Høegreave *et al.*, 1983; Wang, 1986; Robinson, 1988a; 1988b; Combescure, 1992; Arai, 1995; Combescure and Robert, 1997; Robert, 1998], and [Landsman, 1998].

Impressive results are available also in the Schrödinger picture. The counterpart of (17) is that for any suitably smooth classical Hamiltonian  $h$  (even a time-dependent one) that is at most quadratic in the canonical coordinates  $p$  and  $q$  on

<sup>210</sup>More generally, Egorov's Theorem states that for a large class of Hamiltonians one has  $\mathcal{Q}_\hbar^W(f)(t) = \mathcal{Q}_\hbar^W(f_t) + \mathcal{O}(\hbar)$ . See, e.g., [Robert, 1987; Dimassi and Sjöstrand, 1999], and [Martinez, 2002].

<sup>211</sup>Eq. (17) is equivalent to the covariance of Weyl quantization under the affine symplectic group; cf. footnote 153.

phase space  $\mathbb{R}^{2n}$  one may construct generalized coherent states  $\Psi_{(p,q,C)}^{\hbar}$ , labeled by a set  $C$  of classical parameters dictated by the form of  $h$ , such that

$$(21) \quad e^{-\frac{it}{\hbar} \mathcal{Q}_h^W(h)} \Psi_{(p,q,C)}^{\hbar} = e^{iS(t)/\hbar} \Psi_{(p(t),q(t),C(t))}^{\hbar}.$$

Here  $S(t)$  is the action associated with the classical trajectory  $(p(t), q(t))$  determined by  $h$ , and  $C(t)$  is a solution of a certain system of differential equations that has a classical interpretation as well [Hagedorn, 1998]. Schrödinger's coherent states (20) are a special case for the standard harmonic oscillator Hamiltonian. For more general Hamiltonians one then has an asymptotic result [Hagedorn and Joye, 1999; 2000]<sup>212</sup>

$$(22) \quad \lim_{\hbar \rightarrow 0} \left\| e^{-\frac{it}{\hbar} \mathcal{Q}_h^W(h)} \Psi_{(p,q,C)}^{\hbar} - e^{iS(t)/\hbar} \Psi_{(p(t),q(t),C(t))}^{\hbar} \right\| = 0.$$

Once again, at first sight such results merely contribute to the understanding of quantum dynamics in terms of classical motion. As mentioned, they may be converted into statements on the emergence of classical motion from quantum mechanics by taking expectation values of suitable  $\hbar$ -dependent observables of the type  $\mathcal{Q}_h^W(f)$ .

For finite  $\hbar$ , the second term in (22) is a good approximation to the first - the error even being as small as  $\mathcal{O}(\exp(-\gamma/\hbar))$  for some  $\gamma > 0$  as  $\hbar \rightarrow 0$  - whenever  $t$  is smaller than the so-called *Ehrenfest time*

$$(23) \quad T_E = \lambda^{-1} \log(\hbar^{-1}),$$

where  $\lambda$  is a typical inverse time scale of the Hamiltonian (e.g., for chaotic systems it is the largest Lyapunov exponent).<sup>213</sup> This is the typical time scale on which semiclassical approximations to wave packet solutions of the time-dependent Schrödinger equation with a general Hamiltonian tend to be valid [Ehrenfest, 1927; Berry *et al.*, 1979; Zaslavsky, 1981; Combescure and Robert, 1997; Bambusi *et al.*, 1999; Hagedorn and Joye, 2000].<sup>214</sup> For example, Ehrenfest [1927] himself estimated that for a mass of 1 gram a wave packet would double its width only in

<sup>212</sup>See also [Paul and Uribe, 1995; 1996] as well as the references listed after (20) for analogous statements.

<sup>213</sup>Recall that throughout this section we assume that  $\hbar$  has been made dimensionless through an appropriate rescaling.

<sup>214</sup>One should distinguish here between two distinct approximation methods to the time-dependent Schrödinger equation. Firstly, one has the semiclassical propagation of a quantum-mechanical wave packet, i.e. its propagation as computed from the time-dependence of the parameters on which it depends *according to the underlying classical equations of motion*. It is shown in the references just cited that this approximates the full quantum-mechanical propagation of the wave packet well until  $t \sim T_E$ . Secondly, one has the time-dependent WKB approximation (for integrable systems) and its generalization to chaotic systems (which typically involve tens of thousands of terms instead of a single one). This second approximation is valid on a much longer time scale, typically  $t \sim \hbar^{-1/2}$  [O'Connor, Tomsovic, and Heller, 1992; Heller and Tomsovic, 1993; Tomsovic and Heller, 1993; 2002; Vanicek and Heller, 2003]. Adding to the confusion, Ballentine has claimed over the years that even the semiclassical propagation of a wave packet approximates its quantum-mechanical propagation for times much longer than the Ehrenfest time, typically  $t \sim \hbar^{-1/2}$  [Ballentine *et al.*, 1994; Ballentine, 2002; 2003]. This claim

about  $10^{13}$  years under free motion. However, Zurek and Paz [1995] have estimated the Ehrenfest time for Saturn's moon Hyperion to be of the order of 20 years! This obviously poses a serious problem for the program of deriving (the appearance of) classical behaviour from quantum mechanics, which affects all interpretations of this theory.

Finally, we have not discussed the important problem of combining the limit  $t \rightarrow \infty$  with the limit  $\hbar \rightarrow 0$ ; this should be done in such a way that  $T_E$  is kept fixed. This double limit is of particular importance for quantum chaos; see Robert [1998] and most of the literature cited in Subsection 5.6.

### 5.3 Wigner functions

The  $\hbar \rightarrow 0$  limit of quantum mechanics is often discussed in terms of the so-called *Wigner function*, introduced by Wigner [1932].<sup>215</sup> Each unit vector (i.e. wave function)  $\Psi \in L^2(\mathbb{R}^n)$  defines such a function  $W_\Psi^\hbar$  on classical phase space  $M = \mathbb{R}^{2n}$  by demanding that for each  $f \in \mathcal{S}(\mathbb{R}^{2n})$  one has

$$(24) \quad (\Psi, \mathcal{Q}_\hbar^W(f)\Psi) = \int_{\mathbb{R}^{2n}} \frac{d^n p d^n q}{(2\pi)^n} W_\Psi^\hbar(p, q) f(p, q).$$

The existence of such a function may be proved by writing it down explicitly as

$$(25) \quad W_\Psi^\hbar(p, q) = \int_{\mathbb{R}^n} d^n v e^{ipv} \overline{\Psi(q + \frac{1}{2}\hbar v)} \Psi(q - \frac{1}{2}\hbar v).$$

In other words, the quantum-mechanical expectation value of the Weyl quantization of the classical observable  $f$  in a quantum state  $\Psi$  formally equals the classical expectation value of  $f$  with respect to the distribution  $W_\Psi$ . However, the latter may not be regarded as a probability distribution because it is not necessarily positive definite.<sup>216</sup> Despite this drawback, the Wigner function possesses some attractive properties. For example, one has

$$(26) \quad \mathcal{Q}_\hbar^W(W_\Psi^\hbar) = \hbar^{-n} [\Psi].$$

This somewhat perverse result means that if the Wigner function defined by  $\Psi$  is seen as a classical observable (despite its manifest  $\hbar$ -dependence!), then its Weyl

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is based on the criterion that the quantum and classical (i.e. Liouville) probabilities are approximately equal on such time scales, but the validity of this criterion hinges on the “statistical” or “ensemble” interpretation of quantum mechanics. According to this interpretation, a pure state provides a description of certain statistical properties of an ensemble of similarly prepared systems, but need not provide a complete description of an individual system. See [Ballentine, 1970; 1986]. Though once defended by von Neumann, Einstein and Popper, this interpretation has now completely fallen out of fashion.

<sup>215</sup>The original context was quantum statistical mechanics; one may write down (24) for mixed states as well. See [Hillery *et al.*, 1984] for a survey.

<sup>216</sup>Indeed, it may not even be in  $L^1(\mathbb{R}^{2n})$ , so that its total mass is not necessarily defined, let alone equal to 1. Conditions for the positivity of Wigner functions defined by pure states are given by Hudson [1974]; see [Bröcker and Werner, 1995] for the case of mixed states.

quantization is precisely ( $\hbar^{-n}$  times) the projection operator onto  $\Psi$ .<sup>217</sup> Furthermore, one may derive the following formula for the transition probability:<sup>218</sup>

$$(27) \quad |(\Phi, \Psi)|^2 = \hbar^n \int_{\mathbb{R}^{2n}} \frac{d^n p d^n q}{(2\pi)^n} W_{\Psi}^{\hbar}(p, q) W_{\Phi}^{\hbar}(p, q).$$

This expression has immediate intuitive appeal, since the integrand on the right-hand side is supported by the area in phase space where the two Wigner functions overlap, which is well in tune with the idea of a transition probability.

The potential lack of positivity of a Wigner function may be remedied by noting that Berezin's deformation quantization scheme (see (28)) analogously defines functions  $B_{\Psi}^{\hbar}$  on phase space by means of

$$(28) \quad (\Psi, \mathcal{Q}_{\hbar}^B(f)\Psi) = \int_{\mathbb{R}^{2n}} \frac{d^n p d^n q}{(2\pi)^n} B_{\Psi}^{\hbar}(p, q) f(p, q).$$

Formally, (27) and (28) immediately yield

$$(29) \quad B_{\Psi}^{\hbar}(p, q) = \hbar^{-n} |(\Psi_{(p,q)}^{\hbar}, \Psi)|^2$$

in terms of Schrödinger's coherent states (20). This expression is manifestly positive definite. The existence of  $B_{\Psi}^{\hbar}$  may be proved rigorously by recalling that the Berezin quantization map  $f \mapsto \mathcal{Q}_{\hbar}^B(f)$  is *positive* from  $C_0(\mathbb{R}^{2n})$  to  $\mathcal{B}(L^2(\mathbb{R}^n))$ . This implies that for each (unit) vector  $\Psi \in L^2(\mathbb{R}^n)$  the map  $f \mapsto (\Psi, \mathcal{Q}_{\hbar}^B(f)\Psi)$  is positive from  $C_c(\mathbb{R}^{2n})$  to  $\mathbb{C}$ , so that (by the Riesz theorem of measure theory) there must be a measure  $\mu_{\Psi}$  on  $\mathbb{R}^{2n}$  such that  $(\Psi, \mathcal{Q}_{\hbar}^B(f)\Psi) = \int d\mu_{\Psi} f$ . This measure, then, is precisely given by  $d\mu_{\Psi}(p, q) = (2\pi)^{-n} d^n p d^n q B_{\Psi}^{\hbar}(p, q)$ . If  $(\Psi, \Psi) = 1$ , then  $\mu_{\Psi}$  is a probability measure. Accordingly, despite its  $\hbar$ -dependence,  $B_{\Psi}^{\hbar}$  defines a bona fide classical probability distribution on phase space, in terms of which one might attempt to visualize quantum mechanics to some extent.

For finite values of  $\hbar$ , the Wigner and Berezin distribution functions are different, because the quantization maps  $\mathcal{Q}_{\hbar}^W$  and  $\mathcal{Q}_{\hbar}^B$  are. The connection between  $B_{\Psi}^{\hbar}$  and  $W_{\Psi}^{\hbar}$  is easily computed to be

$$(30) \quad B_{\Psi}^{\hbar} = W_{\Psi}^{\hbar} * g^{\hbar},$$

where  $g^{\hbar}$  is the Gaussian function

$$(31) \quad g^{\hbar}(p, q) = (2/\hbar)^n \exp(-(p^2 + q^2)/\hbar).$$

This is how physicists look at the Berezin function,<sup>219</sup> viz. as a Wigner function smeared with a Gaussian so as to become positive. But since  $g^{\hbar}$  converges to a

<sup>217</sup>In other words,  $W_{\Psi}$  is the Weyl symbol of the projection operator  $[\Psi]$ .

<sup>218</sup>This formula is well defined since  $\Psi \in L^2(\mathbb{R}^n)$  implies  $W_{\Psi}^{\hbar} \in L^2(\mathbb{R}^{2n})$ .

<sup>219</sup>The 'Berezin' functions  $B_{\Psi}^{\hbar}$  were introduced by Husimi [1940] from a different point of view, and are therefore actually called *Husimi functions* by physicists.



Dirac delta function as  $\hbar \rightarrow 0$  (with respect to the measure  $(2\pi)^{-n} d^n p d^n q$  in the sense of distributions), it is clear from (30) that as distributions one has<sup>220</sup>

$$(32) \quad \lim_{\hbar \rightarrow 0} (B_{\Psi}^{\hbar} - W_{\Psi}^{\hbar}) = 0.$$

See also (32). Hence in the study of the limit  $\hbar \rightarrow 0$  there is little advantage in the use of Wigner functions; quite to the contrary, in limiting procedures their generic lack of positivity makes them more difficult to handle than Berezin functions.<sup>221</sup> For example, one would like to write the asymptotic behaviour (8) of coherent states in the form  $\lim_{\hbar \rightarrow 0} W_{\Psi_z^{\hbar}}^{\hbar} = \delta_z$ . Although this is indeed true in the sense of distributions, the corresponding limit

$$(33) \quad \lim_{\hbar \rightarrow 0} B_{\Psi_z^{\hbar}}^{\hbar} = \delta_z,$$

exists in the sense of (probability) measures, and is therefore defined on a much larger class of test functions.<sup>222</sup> Here and in what follows, we abuse notation: if  $\mu^0$  is some probability measure on  $\mathbb{R}^{2n}$  and  $(\Psi^{\hbar})$  is a sequence of unit vectors in  $L^2(\mathbb{R}^n)$  indexed by  $\hbar$  (and perhaps other labels), then  $B_{\Psi^{\hbar}}^{\hbar} \rightarrow \mu^0$  for  $\hbar \rightarrow 0$  by definition means that for any  $f \in C_c^{\infty}(\mathbb{R}^{2n})$  one has<sup>223</sup>

$$(34) \quad \lim_{\hbar \rightarrow 0} (\Psi^{\hbar}, \mathcal{Q}_{\hbar}^B(f)\Psi^{\hbar}) = \int_{\mathbb{R}^{2n}} d\mu^0 f.$$

### 5.4 The classical limit of energy eigenstates

Having dealt with coherent states  $\Psi_z^{\hbar}$  in (33), in this subsection we discuss the much more difficult problem of computing the limit measure  $\mu^0$  for eigenstates  $\Psi_n^{\hbar}$  of the quantum Hamiltonian  $H$ . Thus we assume that  $H$  has eigenvalues  $E_n^{\hbar}$  labeled by  $n \in \mathbb{N}$  (defined with or without 0 according to convenience), and also depending on  $\hbar$  because of the explicit dependence of  $H$  on this parameter. The associated eigenstates  $\Psi_n^{\hbar}$  then by definition satisfy

$$(35) \quad H\Psi_n^{\hbar} = E_n^{\hbar}\Psi_n^{\hbar}.$$

Here we incorporate the possibility that the eigenvalue  $E_n^{\hbar}$  is degenerate, so that the label  $n$  extends  $n$ . For example, for the one-dimensional harmonic oscillator one has  $E_n^{\hbar} = \hbar\omega(n + \frac{1}{2})$  ( $n = 0, 1, 2, \dots$ ) without multiplicity, but for the hydrogen

<sup>220</sup> Eq. (32) should be interpreted as a limit of the distribution on  $\mathcal{D}(\mathbb{R}^{2n})$  or  $\mathcal{S}(\mathbb{R}^{2n})$  defined by  $B_{\Psi}^{\hbar} - W_{\Psi}^{\hbar}$ . Both functions are continuous for  $\hbar > 0$ , but lose this property in the limit  $\hbar \rightarrow 0$ , generally converging to distributions.

<sup>221</sup> See, however, [Robinett, 1993] and [Arai, 1995]. It should be mentioned that (32) expresses the asymptotic equivalence of Wigner and Berezin functions as distributions on  $\hbar$ -independent test functions. Even in the limit  $\hbar \rightarrow 0$  one is sometimes interested in studying  $O(\hbar)$  phenomena, in which case one should make a choice.

<sup>222</sup> Namely those in  $C_0(\mathbb{R}^{2n})$  rather than in  $\mathcal{D}(\mathbb{R}^{2n})$  or  $\mathcal{S}(\mathbb{R}^{2n})$ .

<sup>223</sup> Since  $\mathcal{Q}_{\hbar}^B$  may be extended from  $C_c^{\infty}(\mathbb{R}^{2n})$  to  $L^{\infty}(\mathbb{R}^{2n})$ , one may omit the stipulation that  $\mu^0$  be a probability measure in this definition if one requires convergence for all  $f \in L^{\infty}(\mathbb{R}^{2n})$ , or just for all  $f$  in the unitization of the  $C^*$ -algebra  $C_0(\mathbb{R}^{2n})$ .

atom the Bohrian eigenvalues  $E_n^{\hbar} = -m_e e^4 / 2\hbar^2 n^2$  (where  $m_e$  is the mass of the electron and  $e$  is its charge) are degenerate, with the well-known eigenfunctions  $\Psi_{(n,l,m)}^{\hbar}$  [Landau and Lifshitz, 1977]. Hence in this case one has  $\mathfrak{n} = (n, l, m)$  with  $n = 1, 2, 3, \dots$ , subject to  $l = 0, 1, \dots, n - 1$ , and  $m = -l, \dots, l$ .

In any case, it makes sense to let  $\mathfrak{n} \rightarrow \infty$ ; this certainly means  $n \rightarrow \infty$ , and may in addition involve sending the other labels in  $\mathfrak{n}$  to infinity (subject to the appropriate restrictions on  $\mathfrak{n} \rightarrow \infty$ , as above). One then expects classical behaviour à la Bohr if one simultaneously lets  $\hbar \rightarrow 0$  whilst  $E_n^{\hbar} \rightarrow E^0$  converges to some ‘classical’ value  $E^0$ . Depending on how one lets the possible other labels behave in this limit, this may also involve similar asymptotic conditions on the eigenvalues of operators commuting with  $H$  — see below for details in the integrable case. We denote the collection of such eigenvalues (including  $E_n^{\hbar}$ ) by  $E_{\mathfrak{n}}^{\hbar}$ . (Hence in the case where the energy levels  $E_n^{\hbar}$  are nondegenerate, the label  $E$  is just  $E$ .) In general, we denote the collective limit of the eigenvalues  $E_{\mathfrak{n}}^{\hbar}$  as  $\hbar \rightarrow 0$  and  $\mathfrak{n} \rightarrow \infty$  by  $E^0$ .

For example, for the hydrogen atom one has the additional operators  $J^2$  of total angular momentum as well as the operator  $J_3$  of angular momentum in the  $z$ -direction. The eigenfunction  $\Psi_{(n,l,m)}^{\hbar}$  of  $H$  with eigenvalue  $E_n^{\hbar}$  is in addition an eigenfunction of  $J^2$  with eigenvalue  $j_{\hbar}^2 = \hbar^2 l(l + 1)$  and of  $J_3$  with eigenvalue  $j_3^{\hbar} = \hbar m$ . Along with  $n \rightarrow \infty$  and  $\hbar \rightarrow 0$ , one may then send  $l \rightarrow \infty$  and  $m \rightarrow \pm\infty$  in such a way that  $j_{\hbar}^2$  and  $j_3^{\hbar}$  approach specific constants.

The object of interest, then, is the measure on phase space obtained as the limit of the Berezin functions (29), i.e.

$$(36) \quad \mu_E^0 = \lim_{\hbar \rightarrow 0, \mathfrak{n} \rightarrow \infty} B_{\Psi_{\mathfrak{n}}^{\hbar}}.$$

Although the pioneers of quantum mechanics were undoubtedly interested in quantities like this, it was only in the 1970s that rigorous results were obtained. Two cases are well understood: in this subsection we discuss the *integrable* case, leaving chaotic and more generally *ergodic* motion to Subsection 5.6.

In the physics literature, it was argued that for an integrable system the limiting measure  $\mu_E^0$  is concentrated (in the form of a  $\delta$ -function) on the invariant torus associated to  $E^0$  [Berry, 1977a].<sup>224</sup> Independently, mathematicians began to study a quantity very similar to  $\mu_E^0$ , defined by limiting sequences of eigenfunctions of the Laplacian on a Riemannian manifold  $M$ . Here the underlying classical flow is Hamiltonian as well, the corresponding trajectories being the geodesics of the given metric (see, for example, [Klingenberg, 1982; Abraham and Marsden, 1985; Katok and Hasselblatt, 1995], or [Landsman, 1998]).<sup>225</sup> The ensuing picture largely confirms the folklore of the physicists:

*In the integrable case the limit measure  $\mu_E^0$  is concentrated on invariant tori.*

<sup>224</sup>This conclusion was, in fact, reached from the Wigner function formalism. See [Ozorio de Almeida, 1988] for a review of work of Berry and his collaborators on this subject.

<sup>225</sup>The simplest examples of integrable geodesic motion are  $n$ -tori, where the geodesics are projections of lines, and the sphere, where the geodesics are great circles [Katok and Hasselblatt, 1995].

See [Charbonnel, 1986; 1988; Zelditch, 1990, 1996a; Toth, 1996; 1999; Nadirashvili *et al.*, 2001], and [Toth and Zelditch, 2002; 2003a; 2003b].<sup>226</sup> Finally, as part of the transformation of microlocal analysis to semiclassical analysis (cf. Subsection 5.2), these results were adapted to quantum mechanics [Paul and Uribe, 1995; 1996].

Let us now give some details for integrable systems (of Liouville type); these include the hydrogen atom as a special case. Integrable systems are defined by the property that on a  $2p$ -dimensional phase space  $M$  one has  $p$  independent<sup>227</sup> classical observables  $(f_1 = h, f_2, \dots, f_p)$  whose mutual Poisson brackets all vanish [Arnold, 1989]. One then hopes that an appropriate quantization scheme  $\mathcal{Q}_\hbar$  exists under which the corresponding quantum observables  $(\mathcal{Q}_\hbar(f_1) = H, \mathcal{Q}_\hbar(f_2), \dots, \mathcal{Q}_\hbar(f_p))$  are all self-adjoint and mutually commute (on a common core).<sup>228</sup> This is indeed the case for the hydrogen atom, where  $(f_1, f_2, f_3)$  may be taken to be  $(h, j^2, j_3)$  (where  $j^2$  is the total angular momentum and  $j_3$  is its  $z$ -component),<sup>229</sup>  $H$  is given by (16),  $J^2 = \mathcal{Q}_\hbar^W(j^2)$ , and  $J_3 = \mathcal{Q}_\hbar^W(j_3)$ . In general, the energy eigenfunctions  $\Psi_n^\hbar$  will be joint eigenfunctions of the operators  $(\mathcal{Q}_\hbar(f_1), \dots, \mathcal{Q}_\hbar(f_p))$ , so that  $E_n^\hbar = (E_{n_1}^\hbar, \dots, E_{n_p}^\hbar)$ , with  $\mathcal{Q}_\hbar(f_k)\Psi_n^\hbar = E_{n_k}^\hbar \Psi_n^\hbar$ . We assume that the submanifolds  $\cap_{k=1}^p f_k^{-1}(x_k)$  are compact and connected for each  $x \in \mathbb{R}^p$ , so that they are tori by the Liouville–Arnold Theorem [Abraham and Marsden, 1985; Arnold, 1989].

Letting  $\hbar \rightarrow 0$  and  $n \rightarrow \infty$  so that  $E_{n_k}^\hbar \rightarrow E_k^0$  for some point  $E^0 = (E_1^0, \dots, E_p^0) \in \mathbb{R}^p$ , it follows that the limiting measure  $\mu_E^0$  as defined in (36) is concentrated on the invariant torus  $\cap_{k=1}^p f_k^{-1}(E_k^0)$ . This torus is generically  $p$ -dimensional, but for singular points  $E^0$  it may be of lower dimension. In particular, in the exceptional circumstance where the invariant torus is one-dimensional,  $\mu_E^0$  is concentrated on a classical orbit. Of course, for  $p = 1$  (where any Hamiltonian system is integrable) this singular case is generic. Just think of the foliation of  $\mathbb{R}^2$  by the ellipses that form the closed orbits of the harmonic oscillator motion.<sup>230</sup>

<sup>226</sup>These papers consider the limit  $n \rightarrow \infty$  without  $\hbar \rightarrow 0$ ; in fact, a physicist would say that they put  $\hbar = 1$ . In that case  $E_n \rightarrow \infty$ ; in this procedure the physicists' microscopic  $E \sim \mathcal{O}(\hbar)$  and macroscopic  $E \sim \mathcal{O}(1)$  regimes correspond to  $E \sim \mathcal{O}(1)$  and  $E \rightarrow \infty$ , respectively.

<sup>227</sup>I.e.  $df_1 \wedge \dots \wedge df_p \neq 0$  everywhere. At this point we write  $2p$  instead of  $2n$  for the dimension of phase space in order to avoid notational confusion.

<sup>228</sup>There is no general theory of quantum integrable systems. Olshanetsky and Perelomov [1981; 1983] form a good starting point.

<sup>229</sup>In fact, if  $\mu$  is the momentum map for the standard  $SO(3)$ -action on  $\mathbb{R}^3$ , then  $j^2 = \sum_{k=1}^3 \mu_k^2$  and  $j_3 = \mu_3$ .

<sup>230</sup>It may be enlightening to consider geodesic motion on the sphere; this example may be seen as the hydrogen atom without the radial degree of freedom (so that the degeneracy in question occurs in the hydrogen atom as well). If one sends  $l \rightarrow \infty$  and  $m \rightarrow \infty$  in the spherical harmonics  $Y_l^m$  (which are eigenfunctions of the Laplacian on the sphere) in such a way that  $\lim m/l = \cos \varphi$ , then the invariant tori are generically two-dimensional, and occur when  $\cos \varphi \neq \pm 1$ ; an invariant torus labeled by such a value of  $\varphi \neq 0, \pi$  comprises all great circles (regarded as part of phase space by adding to each point of the geodesic a velocity of unit length and direction tangent to the geodesic) whose angle with the  $z$ -axis is  $\varphi$  (more precisely, the angle in question is the one between the normal of the plane through the given great circle and the  $z$ -axis). For  $\cos \varphi = \pm 1$  (i.e.  $m = \pm l$ ), however, there is only one great circle with  $\varphi = 0$  namely the equator (the case

What remains, then, of Bohr's picture of the hydrogen atom in this light?<sup>231</sup> Quite a lot, in fact, confirming his remarkable physical intuition. The energy levels Bohr calculated are those given by the Schrödinger equation, and hence remain correct in mature quantum mechanics. His orbits make literal sense only in the "correspondence principle" limit  $\hbar \rightarrow 0$ ,  $n \rightarrow \infty$ , where, however, the situation is even better than one might expect for integrable systems: because of the high degree of symmetry of the Kepler problem [Guillemin and Sternberg, 1990], one may construct energy eigenfunctions whose limit measure  $\mu^0$  concentrates on any desired classical orbit [Nauenberg, 1989].<sup>232</sup> In order to recover a travelling wave packet, one has to form wave packets from a very large number of energy eigenstates with very high quantum numbers, as explained in Subsection 2.4. For finite  $n$  and  $\hbar$  Bohr's orbits seem to have no meaning, as already recognized by Heisenberg [1969] in his pathfinder days!<sup>233</sup>

### 5.5 The WKB approximation

One might have expected a section on the  $\hbar \rightarrow 0$  limit of quantum mechanics to be centered around the WKB approximation, as practically all textbooks base their discussion of the classical limit on this notion. Although the scope of this method is actually rather limited, it is indeed worth saying a few words about it. For simplicity we restrict ourselves to the time-independent case.<sup>234</sup> In its original formulation, the time-independent WKB method involves an attempt to approximate solutions of the time-independent Schrödinger equation  $H\Psi = E\Psi$  by wave functions of the type

$$(37) \quad \Psi(x) = a_{\hbar}(x)e^{\frac{i}{\hbar}S(x)},$$

where  $a_{\hbar}$  admits an expansion in  $\hbar$  as a power series. Assuming the Hamiltonian  $H$  is of the form (15), plugging the Ansatz (37) into the Schrödinger equation, and expanding in  $\hbar$ , yields in lowest order the classical (time-independent) Hamilton–Jacobi equation

$$(38) \quad h \left( \frac{\partial S}{\partial x}, x \right) = E,$$

---

$\varphi = \pi$  corresponds to the same equator traversed in the opposite direction). Hence in this case the invariant torus is one-dimensional. The reader may be surprised that the invariant tori explicitly depend on the choice of variables, but this feature is typical of so-called degenerate systems; see Arnold (1989), §51.

<sup>231</sup>We ignore coupling to the electromagnetic field here; see footnote 26.

<sup>232</sup>Continuing footnote 230, for a given principal quantum number  $n$  one forms the eigenfunction  $\Psi_{(n,n-1,n-1)}^{\hbar}$  by multiplying the spherical harmonic  $Y_{n-1}^{n-1}$  with the appropriate radial wave function. The limiting measure (36) as  $n \rightarrow \infty$  and  $\hbar \rightarrow 0$  is then concentrated on an orbit (rather than on an invariant torus). Now, beyond what it possible for general integrable systems, one may use the  $SO(4)$  symmetry of the Kepler problem and the construction in footnote 204 for the group-theoretic coherent states of Perelomov [1986] to find the desired eigenfunctions. See also [De Bièvre, 1992] and [De Bièvre *et al.*, 1993].

<sup>233</sup>The later Bohr also conceded this through his idea that causal descriptions are complementary to space-time pictures; see Subsection 3.3.

<sup>234</sup>Cf. [Robert, 1998] and references therein for the time-dependent case.

supplemented by the so-called (homogeneous) transport equation<sup>235</sup>

$$(39) \quad \left( \frac{1}{2} \Delta S + \sum_k \frac{\partial S}{\partial x^k} \frac{\partial}{\partial x^k} \right) a_0 = 0.$$

In particular,  $E$  should be a classically allowed value of the energy. Even when it applies (see below), in most cases of interest the Ansatz (37) is only valid locally (in  $x$ ), leading to problems with caustics. These problems turn out to be an artefact of the use of the coordinate representation that lies behind the choice of the Hilbert space  $\mathcal{H} = L^2(\mathbb{R}^n)$ , and can be avoided [Maslov and Fedoriuk, 1981]: the WKB method really comes to its own in a geometric reformulation in terms of symplectic geometry. See [Arnold, 1989; Bates and Weinstein, 1995], and [Dimassi and Sjöstrand, 1999] for (nicely complementary) introductory treatments, and [Guillemin and Sternberg, 1977; Hörmander, 1985a; 1985b], and [Duistermaat, 1974; 1996] for advanced accounts.

The basic observation leading to this reformulation is that in the rare cases that  $S$  is defined globally as a smooth function on the configuration space  $\mathbb{R}^n$ , it defines a submanifold  $\mathcal{L}$  of the phase space  $M = \mathbb{R}^{2n}$  by  $\mathcal{L} = \{(p = dS(x), q = x), x \in \mathbb{R}^n\}$ . This submanifold is *Lagrangian* in having two defining properties: firstly,  $\mathcal{L}$  is  $n$ -dimensional, and secondly, the restriction of the symplectic form (i.e.  $\sum_k dp_k \wedge dq^k$ ) to  $\mathcal{L}$  vanishes. The Hamilton–Jacobi equation (38) then guarantees that the Lagrangian submanifold  $\mathcal{L} \subset M$  is contained in the surface  $\Sigma_E = h^{-1}(E)$  of constant energy  $E$  in  $M$ . Consequently, any solution of the Hamiltonian equations of motion that starts in  $\mathcal{L}$  remains in  $\mathcal{L}$ .

In general, then, the starting point of the WKB approximation is a Lagrangian submanifold  $\mathcal{L} \subset \Sigma_E \subset M$ , rather than some function  $S$  that defines it locally. By a certain adaptation of the geometric quantization procedure, one may, under suitable conditions, associate a unit vector  $\Psi_{\mathcal{L}}$  in a suitable Hilbert space to  $\mathcal{L}$ , which for small  $\hbar$  happens to be a good approximation to an eigenfunction of  $H$  at eigenvalue  $E$ . This strategy is successful in the integrable case, where the nondegenerate tori (i.e. those of maximal dimension  $n$ ) provide such Lagrangian submanifolds of  $M$ ; the associated unit vector  $\Psi_{\mathcal{L}}$  then turns out to be well defined precisely when  $\mathcal{L}$  satisfies (generalized) Bohr–Sommerfeld quantization conditions. In fact, this is how the measures  $\mu_E^0$  in (36) are generally computed in the integrable case.

If the underlying classical system is not integrable, it may still be close enough to integrability for invariant tori to be defined. Such systems are called quasi-integrable or perturbations of integrable systems, and are described by the Kolmogorov–Arnold–Moser (KAM) theory; see [Gallavotti, 1983; Abraham and Marsden, 1985; Ozorio de Almeida, 1988; Arnold, 1989; Lazutkin, 1993; Gallavotti *et al.*, 2004], and many other books. In such systems the WKB method continues to

<sup>235</sup>Only stated here for a classical Hamiltonian  $h(p, q) = p^2/2m + V(q)$ . Higher-order terms in  $\hbar$  yield further, inhomogeneous transport equations for the expansion coefficients  $a_j(x)$  in  $a_{\hbar} = \sum_j a_j \hbar^j$ . These can be solved in a recursive way, starting with (39).

provide approximations to the energy eigenstates relevant to the surviving invariant tori [Colin de Verdière, 1977; Lazutkin, 1993; Popov, 2000], but already loses some of its appeal.

In general systems, notably chaotic ones, the WKB method is almost useless. Indeed, the following theorem of Werner [1995] shows that the measure  $\mu_E^0$  defined by a WKB function (37) is concentrated on the Lagrangian submanifold  $\mathcal{L}$  defined by  $S$ :

*Let  $a_\hbar$  be in  $L^2(\mathbb{R}^n)$  for each  $\hbar > 0$  with pointwise limit  $a_0 = \lim_{\hbar \rightarrow 0} a_\hbar$  also in  $L^2(\mathbb{R}^n)$ ,<sup>236</sup> and suppose that  $S$  is almost everywhere differentiable. Then for each  $f \in C_c^\infty(\mathbb{R}^{2n})$ :*

$$(40) \quad \lim_{\hbar \rightarrow 0} \left( a_\hbar e^{\frac{i}{\hbar}S}, \mathcal{Q}_\hbar^B(f) a_\hbar e^{\frac{i}{\hbar}S} \right) = \int_{\mathbb{R}^n} d^n x |a_0(x)|^2 f \left( \frac{\partial S}{\partial x}, x \right).$$

As we shall see shortly, this behaviour is impossible for ergodic systems, and this is enough to seal the fate of WKB for chaotic systems in general (except perhaps as a hacker’s tool).

Note, however, that for a given energy level  $E$  the discussion so far has been concerned with properties of the classical trajectories on  $\Sigma_E$  (where they are constrained to remain by conservation of energy). Now, it belongs to the essence of quantum mechanics that other parts of phase space than  $\Sigma_E$  might be relevant to the spectral properties of  $H$  as well. For example, for a classical Hamiltonian of the simple form  $h(p, q) = p^2/2m + V(q)$ , this concerns the so-called *classically forbidden area*  $\{q \in \mathbb{R}^n \mid V(q) > E\}$  (and any value of  $p$ ). Here the classical motion can have no properties like integrability or ergodicity, because it does not exist. Nonetheless, and perhaps counterintuitively, it is precisely here that a slight adaptation of the WKB method tends to be most effective. For  $q = x$  in the classically forbidden area, the Ansatz (37) should be replaced by

$$(41) \quad \Psi(x) = a_\hbar(x) e^{-\frac{S(x)}{\hbar}},$$

where this time  $S$  obeys the Hamilton–Jacobi equation ‘for imaginary time’,<sup>237</sup> i.e.

$$(42) \quad h \left( i \frac{\partial S}{\partial x}, x \right) = E,$$

and the transport equation (39) is unchanged. For example, it follows that in one dimension (with a Hamiltonian of the type (3)) the WKB function (41) assumes the form

$$(43) \quad \Psi(x) \sim e^{-\frac{\sqrt{2m}}{\hbar} \int^{|x|} dy \sqrt{V(y) - E}}$$

<sup>236</sup>This assumption is not made in Werner (1995), who directly assumes that  $\Psi = a_0 \exp(iS/\hbar)$  in (37).

<sup>237</sup>This terminology comes from the Lagrangian formalism, where the classical action  $S = \int dt L(t)$  is replaced by  $iS$  through the substitution  $t = -i\tau$  with  $\tau \in \mathbb{R}$ .

in the forbidden region, which explains both the tunnel effect in quantum mechanics (i.e. the propagation of the wave function into the forbidden region) *and* the fact that this effect disappears in the limit  $\hbar \rightarrow 0$ . However, even here the use of WKB methods has now largely been superseded by techniques developed by Agmon [1982]; see, for example, [Hislop and Sigal, 1996] and [Dimassi and Sjöstrand, 1999] for reviews.

## 5.6 *Epilogue: quantum chaos*

Chaos in classical mechanics was probably known to Newton and was famously highlighted by Poincaré (1892–1899),<sup>238</sup> but its relevance for (and potential threat to) quantum theory was apparently first recognized by Einstein [1917] in a paper that was ‘completely ignored for 40 years’ [Gutzwiller, 1992].<sup>239</sup> Currently, the study of quantum chaos is one of the most thriving businesses in all of physics, as exemplified by innumerable conference proceedings and monographs on the subject, ranging from the classic by Gutzwiller [1990] to the online *opus magnum* by Cvitanovic *et al.* [2005].<sup>240</sup> Nonetheless, the subject is still not completely understood, and provides a fascinating testing ground for the interplay between classical and quantum mechanics.

One should distinguish between various different goals in the field of quantum chaos. The majority of papers and books on quantum chaos is concerned with the semiclassical analysis of some concretely given quantum system having a chaotic system as its classical limit. This means that one tries to approximate (for small  $\hbar$ ) a suitable quantum-mechanical expression in terms of data associated with the underlying classical motion. Michael Berry even described this goal as the “Holy Grail” of quantum chaos. The methods described in Subsection 5.2 contribute to this goal, but are largely independent of the nature of the dynamics. In this subsection we therefore concentrate on techniques and results specific to chaotic motion.

Historically, the first new tool in semiclassical approximation theory that specifically applied to chaotic systems was the so-called *Gutzwiller trace formula*.<sup>241</sup> Roughly speaking, this formula approximates the eigenvalues of the quantum Hamiltonian in terms of the periodic (i.e. closed) orbits of the underlying clas-

<sup>238</sup>See also [Diacu and Holmes, 1996] and [Barrow-Green, 1997] for historical background.

<sup>239</sup>It was the study of the very same Helium atom that led Heisenberg to believe that a fundamentally new ‘quantum’ mechanics was needed to replace the inadequate old quantum theory of Bohr and Sommerfeld. See [Mehra and Rechenberg, 1982b] and [Cassidy, 1992]. Another microscopic example of a chaotic system is the hydrogen atom in an external magnetic field.

<sup>240</sup>Other respectable books include, for example, [Guhr *et al.*, 1998, [Haake, 2001] and [Reichl, 2004].

<sup>241</sup>This attribution is based on Gutzwiller [1971]. A similar result was independently derived by Balian and Bloch [1972; 1974]. See also [Gutzwiller, 1990] and [Brack and Bhaduri, 2003] for mathematically heuristic but otherwise excellent accounts of semiclassical physics based on the trace formula. Mathematically rigorous discussions and proofs may be found in [Colin de Verdière, 1973; Duistermaat and Guillemin, 1975; Guillemin and Uribe, 1989; Paul and Uribe, 1995], and [Combes *et al.*, 1999].

sical Hamiltonian.<sup>242</sup> The Gutzwiller trace formula does not start from the wave function (as the WKB approximation does), but from the *propagator*  $K(x, y, t)$ . Physicists write this as  $K(x, y, t) = \langle x | \exp(-itH/\hbar) | y \rangle$ , whereas mathematicians see it as the Green's function in the formula

$$(44) \quad e^{-\frac{it}{\hbar}H}\Psi(x) = \int d^n y K(x, y, t)\Psi(y),$$

where  $\Psi \in L^2(\mathbb{R}^n)$ . Its (distributional) Laplace transform

$$(45) \quad G(x, y, E) = \frac{1}{i\hbar} \int_0^\infty dt K(x, y, t) e^{\frac{itE}{\hbar}}$$

contains information about both the spectrum and the eigenfunctions; for if the former is discrete, one has

$$(46) \quad G(x, y, E) = \sum_j \frac{\Psi_j(x)\overline{\Psi_j(y)}}{E - E_j}.$$

It is possible to approximate  $K$  or  $G$  itself by an expression of the type

$$(47) \quad K(x, y, t) \sim (2\pi i\hbar)^{-n/2} \sum_P \sqrt{|\det V_P|} e^{\frac{i}{\hbar}S_P(x,y,t) - \frac{1}{2}i\pi\mu_P},$$

where the sum is over *all* classical paths  $P$  from  $y$  to  $x$  in time  $t$  (i.e. paths that solve the classical equations of motion). Such a path has an associated action  $S_P$ , Maslov index  $\mu_P$ , and Van Vleck [1928] determinant  $\det V_P$  [Arnold, 1989]. For chaotic systems one typically has to include tens of thousands of paths in the sum, but if one does so the ensuing approximation turns out to be remarkably successful [Heller and Tomsovic, 1993; Tomsovic and Heller, 1993]. The Gutzwiller trace formula is a semiclassical approximation to

$$(48) \quad g(E) = \int d^n x G(x, x, E) = \sum_j \frac{1}{E - E_j},$$

for a quantum Hamiltonian with discrete spectrum and underlying classical Hamiltonian having chaotic motion. It has the form

$$(49) \quad g(E) \sim g_0(E) + \frac{1}{i\hbar} \sum_P \sum_{k=1}^\infty \frac{T_P}{2 \sinh(k\chi_P/2)} e^{\frac{ik}{\hbar}S_P(E) - \frac{1}{2}i\pi\mu_P},$$

where  $g_0$  is a smooth function giving the mean density of states. This time, the sum is over all (prime) *periodic* paths  $P$  of the classical Hamiltonian at energy  $E$  with associated action  $S_P(E) = \oint pdq$  (where the momentum  $p$  is determined by  $P$ , given  $E$ ), period  $T_P$ , and stability exponent  $\chi_P$  (this is a measure of how rapidly neighbouring trajectories drift away from  $P$ ). Since the frustration expressed by

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<sup>242</sup>Such orbits are dense but of Liouville measure zero in chaotic classical systems. Their crucial role was first recognized by Poincaré (1892–1899).



Einstein [1917], this was the first indication that semiclassical approximations had some bearing on chaotic systems.

Another important development concerning energy levels was the formulation of two key conjectures:<sup>243</sup>

- If the classical dynamics defined by the classical Hamiltonian  $h$  is integrable, then the spectrum of  $H$  is “uncorrelated” or “random” [Berry and Tabor, 1977].
- If the classical dynamics defined by  $h$  is chaotic, then the spectrum of  $H$  is “correlated” or “regular” [Bohigas, Giannoni, and Schmit, 1984].

The notions of correlation and randomness used here can be made precise using notions like the distribution of level spacings and the pair correlation function of eigenvalues; see [Zelditch, 1996a] and [De Bièvre, 2001] for introductory treatments, and most of the literature cited in this subsection for further details.<sup>244</sup>

We now consider energy eigenfunctions instead of eigenvalues, and return to the limit measure (36). In the non (quasi-) integrable case, the key result is that

*for ergodic classical motion,<sup>245</sup> the limit measure  $\mu_E^0$  coincides with the (normalized) Liouville measure induced on the constant energy surface  $\Sigma_E \equiv h^{-1}(E)$ .<sup>246</sup>*

This result was first suggested in the mathematical literature for ergodic geodesic motion on compact hyperbolic Riemannian manifolds [Snirelman, 1974], where it was subsequently proved with increasing generality [Colin de Verdière, 1985; Zelditch, 1987].<sup>247</sup> For certain other ergodic systems this property was proved by Zelditch [1991], Gérard and Leichtnam [1993], Zelditch and Zworski [1996], and

<sup>243</sup>Strictly speaking, both conjectures are wrong; for example, the harmonic oscillator yields a counterexamples to the first one. See [Zelditch, 1996a] for further information. Nonetheless, the conjectures are believed to be true in a deeper sense.

<sup>244</sup>This aspect of quantum chaos has applications to number theory and might even lead to a proof of the Riemann hypothesis; see, for example, [Sarnak, 1999; Berry and Keating, 1999], and many other recent papers. Another relevant connection, related to the one just mentioned, is between energy levels and random matrices; see especially [Guhr *et al.*, 1998]. For the plain relevance of all this to practical physics see [Mirlin, 2000].

<sup>245</sup>Ergodicity is the weakest property that any chaotic dynamical system possesses. See [Katok and Hasselblatt, 1995; Emch and Liu, 2002; Gallavotti *et al.*, 2004], and countless other books.

<sup>246</sup>The unnormalized Liouville measure  $\mu_E^u$  on  $\Sigma_E$  is defined by  $\mu_E^u(B) = \int_B dS_E(x) (\|dh(x)\|)^{-1}$ , where  $dS_E$  is the surface element on  $\Sigma_E$  and  $B \subset \Sigma_E$  is a Borel set. If  $\Sigma_E$  is compact, the normalized Liouville measure  $\mu_E$  on  $\Sigma_E$  is given by  $\mu_E(B) = \mu_E^u(B)/\mu_E^u(\Sigma_E)$ . It is a probability measure on  $\Sigma_E$ , reflecting the fact that the eigenvectors  $\Psi_n^h$  are normalized to unit length so as to define quantum-mechanical states.

<sup>247</sup>In the Riemannian case with  $\hbar = 1$  the cosphere bundle  $S^*Q$  (i.e. the subbundle of the cotangent bundle  $T^*Q$  consisting of one-forms of unit length) plays the role of  $\Sigma_E$ . Low-dimensional examples of ergodic geodesic motion are provided by compact hyperbolic spaces. Also cf. [Zelditch, 1992a] for the physically important case of a particle moving in an external gauge field. See also the appendix to Lazutkin [1993] by A.I. Shnirelman, and [Nadirashvili *et al.*, 2001] for reviews.

others; to the best of our knowledge a completely general proof remains to be given.

An analogous version for Schrödinger operators on  $\mathbb{R}^n$  was independently stated in the physics literature [Berry, 1977b; Voros, 1979], and was eventually proved under certain assumptions on the potential by Helffer, Martinez and Robert [1987], Charbonnel [1992], and Paul and Uribe [1995]. Under suitable assumptions one therefore has

$$(50) \quad \lim_{\hbar \rightarrow 0, n \rightarrow \infty} (\Psi_n^\hbar, \mathcal{Q}_\hbar^B(f)\Psi_n^\hbar) = \int_{\Sigma_E} d\mu_E f$$

for any  $f \in C_c^\infty(\mathbb{R}^{2n})$ , where again  $\mu_E$  is the (normalized) Liouville measure on  $\Sigma_E \subset \mathbb{R}^{2n}$  (assuming this space to be compact). In particular, in the ergodic case  $\mu_E^0$  only depends on  $E^0$  and is the same for (almost) every sequence of energy eigenfunctions  $(\Psi_n^\hbar)$  as long as  $E_n^\hbar \rightarrow E^0$ .<sup>248</sup> Thus the support of the limiting measure is uniformly spread out over the largest part of phase space that is dynamically possible.

The result that for ergodic classical motion  $\mu_E^0$  is the Liouville measure on  $\Sigma_E$  under the stated condition leaves room for the phenomenon of ‘scars’, according to which in chaotic systems the limiting measure is sometimes concentrated on periodic classical orbits. This terminology is used in two somewhat different ways in the literature. ‘Strong’ scars survive in the limit  $\hbar \rightarrow 0$  and concentrate on stable closed orbits;<sup>249</sup> they may come from ‘exceptional’ sequences of eigenfunctions.<sup>250</sup> These are mainly considered in the mathematical literature; cf. [Nadirashvili *et al.*, 2001] and references therein.

In the physics literature, on the other hand, the notion of a scar usually refers to an anomalous concentration of the functions  $B_{\Psi_n^\hbar}^\hbar$  (cf. (29)) near *unstable* closed orbits for *finite* values of  $\hbar$ ; see [Heller and Tomsovic, 1993; Tomsovic and Heller, 1993; Kaplan and Heller, 1998a; 1998b], and [Kaplan, 1999] for surveys. Such scars turn out to be crucial in attempts to explain the energy spectrum of the associated quantum system. The reason why such scars do not survive the (double) limit in (36) is that this limit is defined with respect to  $\hbar$ -independent smooth test functions. Physically, this means that one averages over more and more De Broglie wavelengths as  $\hbar \rightarrow 0$ , eventually losing information about the single wavelength scale [Kaplan, 1999]. Hence to pick them up in a mathematically sound way, one should redefine (36) as a pointwise limit [Duclos and Hogreve, 1993; Paul and Uribe, 1996; 1998]. In any case, there is no contradiction between the mathematical results cited and what physicists have found.

Another goal of quantum chaos is the identification of chaotic phenomena within a given quantum-mechanical model. Here the slight complication arises that one

<sup>248</sup> The result is not necessarily valid for all sequences  $(\Psi_n^\hbar)$  with the given limiting behaviour, but only for ‘almost all’ such sequences (technically, for a class of sequences of density 1). See, for example, [De Bièvre, 2001] for a simple explanation of this.

<sup>249</sup> An orbit  $\gamma \subset M$  is called *stable* when for each neighbourhood  $U$  of  $\gamma$  there is neighbourhood  $V \subset U$  of  $\gamma$  such that  $z(t) \in U$  for all  $z \in V$  and all  $t$ .

<sup>250</sup> Cf. footnote 248.

cannot simply copy the classical definition of chaos in terms of diverging trajectories in phase space, since (by unitarity of time-evolution) in quantum mechanics  $\|\Psi(t) - \Phi(t)\|$  is constant in time  $t$  for solutions of the Schrödinger equation. However, this just indicates that should intrinsic quantum chaos exist, it has to be defined differently from classical chaos.<sup>251</sup> This has now been largely accomplished in the algebraic formulation of quantum theory [Benatti, 1993; Emch *et al.*, 1994; Zelditch, 1996b; 1996c; Belot and Earman, 1997; Alicki and Fannes, 2001; Narnhofer, 2001]. The most significant recent development in this direction in the “heuristic” literature has been the study of the quantity

$$(51) \quad M(t) = |(e^{-\frac{it}{\hbar}(H+\Sigma)}\Psi, e^{-\frac{it}{\hbar}H}\Psi)|^2,$$

where  $\Psi$  is a coherent state (or Gaussian wave packet), and  $\Sigma$  is some perturbation of the Hamiltonian  $H$  [Peres, 1984]. In what is generally regarded as a breakthrough in the field, Jalabert and Pastawski [2001] discovered that in a certain regime  $M(t)$  is independent of the detailed form of  $\Sigma$  and decays as  $\sim \exp(-\lambda t)$ , where  $\lambda$  is the (largest) Lyapunov exponent of the underlying classical system. See [Cucchietti, 2004] for a detailed account and further development.

In any case, the possibility that classical chaos appears in the  $\hbar \rightarrow 0$  limit of quantum mechanics is by no means predicated on the existence of intrinsic quantum chaos in the above sense.<sup>252</sup> For even in the unlikely case that quantum dynamics would turn out to be intrinsically non-chaotic, its classical limit is sufficiently singular to admit kinds of classical motion without a qualitative counterpart in quantum theory. This possibility is not only confirmed by most of the literature on quantum chaos (little of which makes any use of notions of intrinsic quantum chaotic motion), but even more so by the possibility of *incomplete* motion. This is a type of dynamics in which the flow of the Hamiltonian vector field is only defined until a certain time  $t_f < \infty$  (or from an initial time  $t_i > -\infty$ ), which means that the equations of motion have no solution for  $t > t_f$  (or  $t < t_i$ ).<sup>253</sup> The

<sup>251</sup>As pointed out by Belot and Earman [1997], the Koopman formulation of classical mechanics (cf. footnote 172) excludes classical chaos if this is formulated in terms of trajectories in Hilbert space. The transition from classical to quantum notions of chaos can be smoothed by first reformulating the classical definition of chaos (normally put in terms of properties of trajectories in phase space).

<sup>252</sup>Arguments by [Ford, 1988] and others to the effect that quantum mechanics is wrong because it cannot give rise to chaos in its classical limit have to be discarded for the reasons given here. See also [Belot and Earman, 1997]. In fact, using the same argument, such authors could simultaneously have ‘proved’ the *opposite* statement that any classical dynamics that arises as the classical limit of a quantum theory with non-degenerate spectrum must be ergodic. For the naive definition of quantum ergodic flow clearly is that quantum time-evolution sweeps out all states at some energy  $E$ ; but for non-degenerate spectra this is a tautology by definition of an eigenfunction!

<sup>253</sup>The simplest examples are incomplete Riemannian manifolds  $Q$  with geodesic flow; within this class, the case  $Q = (0, 1)$  with flat metric is hard to match in simplicity. Clearly, the particle reaches one of the two boundary points in finite time, and does not know what to do (or even whether it exists) afterwards. Other examples come from potentials  $V$  on  $Q = \mathbb{R}^n$  with the property that the classical dynamics is incomplete; see [Reed and Simon, 1975] and [Gallavotti, 1983]. On a somewhat different note, the Universe itself has incomplete dynamics because of the Big Bang and possible Big Crunch.

point, then, is that unitary quantum dynamics, though intrinsically complete, may very well have incomplete motion as its classical limit.<sup>254</sup>

## 6 THE LIMIT $N \rightarrow \infty$

In this section we show to what extent classical physics may approximately emerge from quantum theory when the size of a system becomes large. Strictly classical behaviour would be an idealization reserved for the limit where this size is infinite, which we symbolically denote by “ $\lim N \rightarrow \infty$ ”. As we shall see, mathematically speaking this limit is a special case of the limit  $\hbar \rightarrow 0$  discussed in the previous chapter. What is more, we shall show that formally the limit  $N \rightarrow \infty$  even falls under the heading of continuous fields of  $C^*$ -algebras and deformation quantization (see Subsection 4.3.) Thus the ‘philosophical’ nature of the idealization involved in assuming that a system is infinite is much the same as that of assuming  $\hbar \rightarrow 0$  in a quantum system of given (finite) size; in particular, the introductory comments in Section 1 apply here as well.

An analogous discussion pertains to the derivation of thermodynamics from statistical mechanics [Emch and Liu, 2002; Batterman, 2005]. For example, *in theory* phase transitions only occur in infinite systems, but *in practice* one sees them every day. Thus it appears to be valid to approximate a pot of  $10^{23}$  boiling water molecules by an infinite number of such molecules. The basic point is that the distinction between microscopic and macroscopic regimes is unsharp unless one admits infinite systems as an idealization, so that one can simply say that

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<sup>254</sup> The quantization of the Universe is unknown at present, but geodesic motion on Riemannian manifolds, complete or not, is quantized by  $H = -\frac{\hbar^2}{2m}\Delta$  (perhaps with an additional term proportional to the Ricci scalar  $R$ , see [Landsman, 1998]), where  $\Delta$  is the Laplacian, and quantization on  $Q = \mathbb{R}^n$  is given by the Schrödinger equation (3), whether or not the classical dynamics is complete. In these two cases, and probably more generally, the incompleteness of the classical motion is often (but not always) reflected by the lack of essential self-adjointness of the quantum Hamiltonian on its natural initial domain  $C_c^\infty(Q)$ . For example, if  $Q$  is complete as a Riemannian manifold, then  $\Delta$  is essentially self-adjoint on  $C_c^\infty(Q)$  [Chernoff, 1973; Strichartz, 1983], and if  $Q$  is incomplete then the Laplacian usually fails to be essentially self-adjoint on this domain (but see [Horowitz and Marolf, 1995] for counterexamples). One may refer to the latter property as quantum-mechanical incompleteness [Reed and Simon, 1975], although a Hamiltonian that fails to be essentially self-adjoint on  $C_c^\infty(Q)$  can often be extended (necessarily in a non-unique way) to a self-adjoint operator by a choice of boundary conditions (possibly at infinity). By Stone’s theorem, the quantum dynamics defined by each self-adjoint extension is unitary (and therefore defined for all times). Similarly, although no general statement can be made relating (in)complete classical motion in a potential to (lack of) essential selfadjointness of the corresponding Schrödinger operator, it is usually the case that completeness implies essential selfadjointness, and vice versa. See [Reed and Simon, 1975], Appendix to §X.1, where the reader may also find examples of classically incomplete but quantum-mechanically complete motion, and vice versa. Now, here is the central point for the present discussion: as probably first noted by Hepp [1974], *different self-adjoint extensions have the same classical limit* (in the sense of (20) or similar criteria), namely the given *incomplete* classical dynamics. This proves that complete quantum dynamics can have incomplete motion as its classical limit. However, much remains to be understood in this area. See also [Earman, 2005; 2006].

microscopic systems are finite, whereas macroscopic systems are infinite. This procedure is eventually justified by the results it produces.

Similarly, in the context of quantum theory classical behaviour is simply not found in finite systems (when  $\hbar > 0$  is fixed), whereas, as we shall see, it *is* found in infinite ones. Given the observed classical nature of the macroscopic world,<sup>255</sup> at the end of the day one concludes that the idealization in question is apparently a valid one. One should not be confused by the fact that the error in the number of particles this approximation involves (viz.  $\infty - 10^{23} = \infty$ ) is considerably larger than the number of particles in the actual system. If all of the  $10^{23}$  particles in question were *individually* tracked down, the approximation is indeed a worthless one, but the point is rather that the limit  $N \rightarrow \infty$  is valid whenever *averaging* over  $N = 10^{23}$  particles is well approximated by averaging over an arbitrarily larger number  $N$  (which, then, one might as well let go to infinity). Below we shall give a precise version of this argument.

Despite our opening comments above, the quantum theory of infinite systems has features of its own that deserve a separate section. Our treatment is complementary to texts such as Thirring [1983], Strocchi [1985], Bratteli and Robinson [1987], Haag [1992], Araki [1999], and Sewell [1986; 2002], which should be consulted for further information on infinite quantum systems. The theory in Subsections 6.1 and 6.5 is a reformulation in terms of continuous field of  $C^*$ -algebras and deformation quantization of the more elementary parts of a remarkable series of papers on so-called quantum mean-field systems by Raggio and Werner [1989; 1991], Duffield and Werner [1992a,b,c], and Duffield, Roos, and Werner [1992]. These models have their origin in the treatment of the BCS theory of superconductivity due to Bogoliubov [1958] and Haag [1962], with important further contributions by Thirring and Wehrl [1967], Thirring [1968], Hepp [1972], Hepp and Lieb [1973], Rieckers [1984], Morchio and Strocchi [1987], Duffner and Rieckers [1988], Bona [1988; 1989; 2000], Unnerstall [1990a; 1990b], Bagarello and Morchio [1992], Sewell [2002], and others.

### 6.1 Macroscopic observables

The large quantum systems we are going to study consist of  $N$  copies of a single quantum system with unital algebra of observables  $\mathcal{A}_1$ . Almost all features already emerge in the simplest example  $\mathcal{A}_1 = M_2(\mathbb{C})$  (i.e. the complex  $2 \times 2$  matrices), so there is nothing wrong with having this case in mind as abstraction increases.<sup>256</sup> The aim of what follows is to describe in what precise sense macroscopic observables (i.e. those obtained by averaging over an infinite number of sites) are “classical”.

<sup>255</sup>With the well-known mesoscopic exceptions [Leggett, 2002; Brezger *et al.*, 2002; Chiorescu *et al.*, 2003; Marshall *et al.*, 2003; Devoret *et al.*, 2004].

<sup>256</sup>In the opposite direction of greater generality, it is worth noting that the setting below actually incorporates quantum systems defined on general lattices in  $\mathbb{R}^n$  (such as  $\mathbb{Z}^n$ ). For one could relabel things so as to make  $\mathcal{A}_{1/N}$  below the algebra of observables of all lattice points  $\Lambda$  contained in, say, a sphere of radius  $N$ . The limit  $N \rightarrow \infty$  then corresponds to the limit  $\Lambda \rightarrow \mathbb{Z}^n$ .

From the single  $C^*$ -algebra  $\mathcal{A}_1$ , we construct a continuous field of  $C^*$ -algebras  $\mathcal{A}^{(c)}$  over

$$(1) \quad I = 0 \cup 1/\mathbb{N} = \{0, \dots, 1/N, \dots, \frac{1}{3}, \frac{1}{2}, 1\} \subset [0, 1],$$

as follows. We put

$$(2) \quad \begin{aligned} \mathcal{A}_0^{(c)} &= C(\mathcal{S}(\mathcal{A}_1)); \\ \mathcal{A}_{1/N}^{(c)} &= \mathcal{A}_1^N, \end{aligned}$$

where  $\mathcal{S}(\mathcal{A}_1)$  is the state space of  $\mathcal{A}_1$  (equipped with the weak\*-topology)<sup>257</sup> and  $\mathcal{A}_1^N = \hat{\otimes}^N \mathcal{A}_1$  is the (spatial) tensor product of  $N$  copies of  $\mathcal{A}_1$ .<sup>258</sup> This explains the suffix  $c$  in  $\mathcal{A}^{(c)}$ : it refers to the fact that the limit algebra  $\mathcal{A}_0^{(c)}$  is classical or commutative.

For example, take  $\mathcal{A}_1 = M_2(\mathbb{C})$ . Each state is given by a density matrix, which is of the form

$$(3) \quad \rho(x, y, z) = \frac{1}{2} \begin{pmatrix} 1+z & x-iy \\ x+iy & 1-z \end{pmatrix},$$

for some  $(x, y, z) \in \mathbb{R}^3$  satisfying  $x^2 + y^2 + z^2 \leq 1$ . Hence  $\mathcal{S}(M_2(\mathbb{C}))$  is isomorphic (as a compact convex set) to the three-ball  $B^3$  in  $\mathbb{R}^3$ . The pure states are precisely the points on the boundary,<sup>259</sup> i.e. the density matrices for which  $x^2 + y^2 + z^2 = 1$  (for these and these alone define one-dimensional projections).<sup>260</sup>

In order to define the continuous sections of the field, we introduce the *symmetrization maps*  $j_{NM} : \mathcal{A}_1^M \rightarrow \mathcal{A}_1^N$ , defined by

$$(4) \quad j_{NM}(A_M) = S_N(A_M \otimes 1 \otimes \dots \otimes 1),$$

where one has  $N - M$  copies of the unit  $1 \in \mathcal{A}_1$  so as to obtain an element of  $\mathcal{A}_1^N$ . The symmetrization operator  $S_N : \mathcal{A}_1^N \rightarrow \mathcal{A}_1^N$  is given by (linear and continuous)

<sup>257</sup>In this topology one has  $\omega_\lambda \rightarrow \omega$  when  $\omega_\lambda(A) \rightarrow \omega(A)$  for each  $A \in \mathcal{A}_1$ .

<sup>258</sup>When  $\mathcal{A}_1$  is finite-dimensional the tensor product is unique. In general, one needs the *projective* tensor product at this point. See footnote 90. The point is the same here: any tensor product state  $\omega_1 \otimes \dots \otimes \omega_N$  on  $\hat{\otimes}^N \mathcal{A}_1$  — defined on elementary tensors by  $\omega_1 \otimes \dots \otimes \omega_N(A_1 \otimes \dots \otimes A_N) = \omega_1(A_1) \dots \omega_N(A_N)$  — extends to a state on  $\hat{\otimes}^N \mathcal{A}_1$  by continuity.

<sup>259</sup>The *extreme boundary*  $\partial_e K$  of a convex set  $K$  consists of all  $\omega \in K$  for which  $\omega = p\rho + (1-p)\sigma$  for some  $p \in (0, 1)$  and  $\rho, \sigma \in K$  implies  $\rho = \sigma = \omega$ . If  $K = \mathcal{S}(\mathcal{A})$  is the state space of a  $C^*$ -algebra  $\mathcal{A}$ , the extreme boundary consists of the pure states on  $\mathcal{A}$  (the remainder of  $\mathcal{S}(\mathcal{A})$  consisting of mixed states). If  $K$  is embedded in a vector space, the extreme boundary  $\partial_e K$  may or may not coincide with the geometric boundary  $\partial K$  of  $K$ . In the case  $K = B^3 \subset \mathbb{R}^3$  it does, but for an equilateral triangle in  $\mathbb{R}^2$  it does not, since  $\partial_e K$  merely consists of the corners of the triangle whereas the geometric boundary includes the sides as well.

<sup>260</sup>Eq. (3) has the form  $\rho(x, y, z) = \frac{1}{2}(x\sigma_x + y\sigma_y + z\sigma_z)$ , where the  $\sigma_i$  are the Pauli matrices. This yields an isomorphism between  $\mathbb{R}^3$  and the Lie algebra of  $SO(3)$  in its spin- $\frac{1}{2}$  representation  $\mathcal{D}_{1/2}$  on  $\mathbb{C}^2$ . This isomorphism intertwines the defining action of  $SO(3)$  on  $\mathbb{R}^3$  with its adjoint action on  $M_2(\mathbb{C})$ . I.e., for any rotation  $R$  one has  $\rho(R\mathbf{x}) = \mathcal{D}_{1/2}(R)\rho(\mathbf{x})\mathcal{D}_{1/2}(R)^{-1}$ . This will be used later on (see Subsection 6.5).

extension of

$$(5) \quad S_N(B_1 \otimes \cdots \otimes B_N) = \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_N} B_{\sigma(1)} \otimes \cdots \otimes B_{\sigma(N)},$$

where  $\mathfrak{S}_N$  is the permutation group (i.e. symmetric group) on  $N$  elements and  $B_i \in \mathcal{A}_1$  for all  $i = 1, \dots, N$ . For example,  $j_{N1} : \mathcal{A}_1 \rightarrow \mathcal{A}_1^N$  is given by

$$(6) \quad j_{N1}(B) = \overline{B}^{(N)} = \frac{1}{N} \sum_{k=1}^N 1 \otimes \cdots \otimes B_{(k)} \otimes 1 \cdots \otimes 1,$$

where  $B_{(k)}$  is  $B$  seen as an element of the  $k$ 'th copy of  $\mathcal{A}_1$  in  $\mathcal{A}_1^N$ . As our notation  $\overline{B}^{(N)}$  indicates, this is just the ‘average’ of  $B$  over all copies of  $\mathcal{A}_1$ . More generally, in forming  $j_{NM}(A_M)$  an operator  $A_M \in \mathcal{A}_1^M$  that involves  $M$  sites is averaged over  $N \geq M$  sites. When  $N \rightarrow \infty$  this means that one forms a *macroscopic* average of an  $M$ -particle operator.

We say that a sequence  $A = (A_1, A_2, \dots)$  with  $A_N \in \mathcal{A}_1^N$  is *symmetric* when

$$(7) \quad A_N = j_{NM}(A_M)$$

for some fixed  $M$  and all  $N \geq M$ . In other words, the tail of a symmetric sequence entirely consists of ‘averaged’ or ‘intensive’ observables, which become macroscopic in the limit  $N \rightarrow \infty$ . Such sequences have the important property that they commute in this limit; more precisely, if  $A$  and  $A'$  are symmetric sequences, then

$$(8) \quad \lim_{N \rightarrow \infty} \|A_N A'_N - A'_N A_N\| = 0.$$

As an enlightening special case we take  $A_N = j_{N1}(B)$  and  $A'_N = j_{N1}(C)$  with  $B, C \in \mathcal{A}_1$ . One immediately obtains from the relation  $[B_{(k)}, C_{(l)}] = 0$  for  $k \neq l$  that

$$(9) \quad [\overline{B}^{(N)}, \overline{C}^{(N)}] = \frac{1}{N} \overline{[B, C]}^{(N)}.$$

For example, if  $\mathcal{A}_1 = M_2(\mathbb{C})$  and if for  $B$  and  $C$  one takes the spin- $\frac{1}{2}$  operators  $S_j = \frac{\hbar}{2} \sigma_j$  for  $j = 1, 2, 3$  (where  $\sigma_j$  are the Pauli matrices), then

$$(10) \quad [\overline{S}_j^{(N)}, \overline{S}_k^{(N)}] = i \frac{\hbar}{N} \epsilon_{jkl} \overline{S}_l^{(N)}.$$

This shows that averaging one-particle operators leads to commutation relations formally like those of the one-particle operators in question, but with Planck’s constant  $\hbar$  replaced by a variable  $\hbar/N$ . For constant  $\hbar = 1$  this leads to the interval (1) over which our continuous field of  $C^*$ -algebras is defined; for any other constant value of  $\hbar$  the field would be defined over  $I = 0 \cup \hbar/\mathbb{N}$ , which of course merely changes the labeling of the  $C^*$ -algebras in question.

We return to the general case, and denote a section of the field with fibers (2) by a sequence  $A = (A_0, A_1, A_2, \dots)$ , with  $A_0 \in \mathcal{A}_0^{(c)}$  and  $A_N \in \mathcal{A}_1^N$  as before

(i.e. the corresponding section is  $0 \mapsto A_0$  and  $1/N \mapsto A_N$ ). We then complete the definition of our continuous field by declaring that a sequence  $A$  defines a *continuous* section iff:

- $(A_1, A_2, \dots)$  is *approximately symmetric*, in the sense that for any  $\varepsilon > 0$  there is an  $N_\varepsilon$  and a symmetric sequence  $A'$  such that  $\|A_N - A'_N\| < \varepsilon$  for all  $N \geq N_\varepsilon$ ,<sup>261</sup>
- $A_0(\omega) = \lim_{N \rightarrow \infty} \omega^N(A_N)$ , where  $\omega \in \mathcal{S}(A_1)$  and  $\omega^N \in \mathcal{S}(A_1^N)$  is the tensor product of  $N$  copies of  $\omega$ , defined by (linear and continuous) extension of

$$(11) \quad \omega^N(B_1 \otimes \dots \otimes B_N) = \omega(B_1) \cdots \omega(B_N).$$

This limit exists by definition of an approximately symmetric sequence.<sup>262</sup>

It is not difficult to prove that this choice of continuous sections indeed defines a continuous field of  $C^*$ -algebras over  $I = 0 \cup 1/\mathbb{N}$  with fibers (2). The main point is that

$$(12) \quad \lim_{N \rightarrow \infty} \|A_N\| = \|A_0\|$$

whenever  $(A_0, A_1, A_2, \dots)$  satisfies the two conditions above.<sup>263</sup> This is easy to show for symmetric sequences,<sup>264</sup> and follows from this for approximately symmetric ones.

Consistent with (8), we conclude that in the limit  $N \rightarrow \infty$  the macroscopic observables organize themselves in a commutative  $C^*$ -algebra isomorphic to  $C(\mathcal{S}(A_1))$ .

### 6.2 QuasilocaI observables

In the  $C^*$ -algebraic approach to quantum theory, infinite systems are usually described by means of inductive limit  $C^*$ -algebras and the associated quasilocaI

<sup>261</sup>A symmetric sequence is evidently approximately symmetric.  
<sup>262</sup>If  $(A_1, A_2, \dots)$  is symmetric with (7), one has  $\omega^N(A_N) = \omega^M(A_M)$  for  $N > M$ , so that the tail of the sequence  $(\omega^N(A_N))$  is even independent of  $N$ . In the approximately symmetric case one easily proves that  $(\omega^N(A_N))$  is a Cauchy sequence.  
<sup>263</sup>Given (12), the claim follows from Prop. II.1.2.3 in Landsman [1998] and the fact that the set of functions  $A_0$  on  $\mathcal{S}(A_1)$  arising in the said way are dense in  $C(\mathcal{S}(A_1))$  (equipped with the supremum-norm). This follows from the Stone–Weierstrass theorem, from which one infers that the functions in question even exhaust  $\mathcal{S}(A_1)$ .  
<sup>264</sup>Assume (7), so that  $\|A_N\| = \|j_{NN}(A_N)\|$  for  $N \geq M$ . By the  $C^*$ -axiom  $\|A^*A\| = \|A\|^2$  it suffices to prove (12) for  $A_0^* = A_0$ , which implies  $A_M^* = A_M$  and hence  $A_N^* = A_N$  for all  $N \geq M$ . One then has  $\|A_N\| = \sup\{|\rho(A_N)|, \rho \in \mathcal{S}(A_1^N)\}$ . Because of the special form of  $A_N$  one may replace the supremum over the set  $\mathcal{S}(A_1^N)$  of all states on  $A_1^N$  by the supremum over the set  $\mathcal{S}^p(A_1^N)$  of all permutation invariant states, which in turn may be replaced by the supremum over the extreme boundary  $\partial\mathcal{S}^p(A_1^N)$  of  $\mathcal{S}^p(A_1^N)$ . It is well known ([Størmer, 1969]; see also Subsection 6.2) that the latter consists of all states of the form  $\rho = \omega^N$ , so that  $\|A_N\| = \sup\{|\omega^N(A_N)|, \omega \in \mathcal{S}(A_1)\}$ . This is actually equal to  $\|A_M\| = \sup\{|\omega^M(A_M)|\}$ . Now the norm in  $\mathcal{A}_0^{(c)}$  is  $\|A_0\| = \sup\{|A_0(\omega)|, \omega \in \mathcal{S}(A_1)\}$ , and by definition of  $A_0$  one has  $A_0(\omega) = \omega^M(A_M)$ . Hence (12) follows.



observables [Thirring, 1983; Strocchi, 1985; Bratteli and Robinson, 1981; 1987; Haag, 1992; Araki, 1999; Sewell, 1986; 2002]. To arrive at these notions in the case at hand, we proceed as follows [Duffield and Werner, 1992c].

A sequence  $A = (A_1, A_2, \dots)$  (where  $A_N \in \mathcal{A}_1^N$ , as before) is called *local* when for some fixed  $M$  and all  $N \geq M$  one has  $A_N = A_M \otimes 1 \otimes \dots \otimes 1$  (where one has  $N - M$  copies of the unit  $1 \in \mathcal{A}_1$ ); cf. (4). A sequence is said to be *quasiloca*l when for any  $\varepsilon > 0$  there is an  $N_\varepsilon$  and a local sequence  $A'$  such that  $\|A_N - A'_N\| < \varepsilon$  for all  $N \geq N_\varepsilon$ . On this basis, we define the *inductive limit*  $C^*$ -algebra

$$(13) \quad \overline{\cup_{N \in \mathbb{N}} \mathcal{A}_1^N}$$

of the family of  $C^*$ -algebras  $(\mathcal{A}_1^N)$  with respect to the inclusion maps  $\mathcal{A}_1^N \hookrightarrow \mathcal{A}_1^{N+1}$  given by  $A_N \mapsto A_N \otimes 1$ . As a set, (13) consists of all equivalence classes  $[A] \equiv A_0$  of quasilocal sequences  $A$  under the equivalence relation  $A \sim B$  when  $\lim_{N \rightarrow \infty} \|A_N - B_N\| = 0$ . The norm on  $\overline{\cup_{N \in \mathbb{N}} \mathcal{A}_1^N}$  is

$$(14) \quad \|A_0\| = \lim_{N \rightarrow \infty} \|A_N\|,$$

and the rest of the  $C^*$ -algebraic structure is inherited from the quasilocal sequences in the obvious way (e.g.,  $A_0^* = [A^*]$  with  $A^* = (A_1^*, A_2^*, \dots)$ , etc.). As the notation suggests, each  $\mathcal{A}_1^N$  is contained in  $\overline{\cup_{N \in \mathbb{N}} \mathcal{A}_1^N}$  as a  $C^*$ -subalgebra by identifying  $A_N \in \mathcal{A}_1^N$  with the local (and hence quasilocal) sequence  $A = (0, \dots, 0, A_N \otimes 1, A_N \otimes 1 \otimes 1, \dots)$ , and forming its equivalence class  $A_0$  in  $\overline{\cup_{N \in \mathbb{N}} \mathcal{A}_1^N}$  as just explained.<sup>265</sup> The assumption underlying the common idea that (13) is “the” algebra of observables of the infinite system under study is that by locality or some other human limitation the infinite tail of the system is not accessible, so that the observables must be arbitrarily close (i.e. in norm) to operators of the form  $A_N \otimes 1 \otimes 1, \dots$  for some *finite*  $N$ .

This leads us to a second continuous field of  $C^*$ -algebras  $\mathcal{A}^{(q)}$  over  $0 \cup 1/\mathbb{N}$ , with fibers

$$(15) \quad \begin{aligned} \mathcal{A}_0^{(q)} &= \overline{\cup_{N \in \mathbb{N}} \mathcal{A}_1^N}; \\ \mathcal{A}_{1/N}^{(q)} &= \mathcal{A}_1^N. \end{aligned}$$

Thus the suffix  $q$  reminds one of that fact that the limit algebra  $\mathcal{A}_0^{(q)}$  consists of quasilocal or quantum-mechanical observables. We equip the collection of  $C^*$ -algebras (15) with the structure of a continuous field of  $C^*$ -algebras  $\mathcal{A}^{(q)}$  over  $0 \cup 1/\mathbb{N}$  by declaring that the continuous sections are of the form  $(A_0, A_1, A_2, \dots)$  where  $(A_1, A_2, \dots)$  is quasilocal and  $A_0$  is defined by this quasilocal sequence as just explained.<sup>266</sup> For  $N < \infty$  this field has the same fibers

$$(16) \quad \mathcal{A}_{1/N}^{(q)} = \mathcal{A}_{1/N}^{(c)} = \mathcal{A}_1^N$$

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<sup>265</sup>Of course, the entries  $A_1, \dots, A_{N-1}$ , which have been put to zero, are arbitrary.  
<sup>266</sup>The fact that this defines a continuous field follows from (14) and Prop. II.1.2.3 in [Landsman, 1998]; cf. footnote 263.

as the continuous field  $\mathcal{A}$  of the previous subsection, but the fiber  $\mathcal{A}_0^{(q)}$  is completely different from  $\mathcal{A}_0^{(c)}$ . In particular, if  $\mathcal{A}_1$  is noncommutative then so is  $\mathcal{A}_0^{(q)}$ , for it contains all  $\mathcal{A}_1^N$ .

The relationship between the continuous fields of  $C^*$ -algebras  $\mathcal{A}^{(q)}$  and  $\mathcal{A}^{(c)}$  may be studied in two different (but related) ways. First, we may construct concrete representations of all  $C^*$ -algebras  $\mathcal{A}_1^N$ ,  $N < \infty$ , as well as of  $\mathcal{A}_0^{(c)}$  and  $\mathcal{A}_0^{(q)}$  on a single Hilbert space; this approach leads to superselections rules in the traditional sense. This method will be taken up in the next subsection. Second, we may look at those families of states  $(\omega_1, \omega_{1/2}, \dots, \omega_{1/N}, \dots)$  (where  $\omega_{1/N}$  is a state on  $\mathcal{A}_1^N$ ) that admit limit states  $\omega_0^{(c)}$  and  $\omega_0^{(q)}$  on  $\mathcal{A}_0^{(c)}$  and  $\mathcal{A}_0^{(q)}$ , respectively, such that the ensuing families of states  $(\omega_0^{(c)}, \omega_1, \omega_{1/2}, \dots)$  and  $(\omega_0^{(q)}, \omega_1, \omega_{1/2}, \dots)$  are *continuous* fields of states on  $\mathcal{A}^{(c)}$  and on  $\mathcal{A}^{(q)}$ , respectively (cf. the end of Subsection 5.1).

Now, any state  $\omega_0^{(q)}$  on  $\mathcal{A}_0^{(q)}$  defines a state  $\omega_{0|1/N}^{(q)}$  on  $\mathcal{A}_1^N$  by restriction, and the ensuing field of states on  $\mathcal{A}^{(q)}$  is clearly continuous. Conversely, any continuous field  $(\omega_0^{(q)}, \omega_1, \omega_{1/2}, \dots, \omega_{1/N}, \dots)$  of states on  $\mathcal{A}^{(q)}$  becomes arbitrarily close to a field of the above type for  $N$  large.<sup>267</sup> However, the restrictions  $\omega_{0|1/N}^{(q)}$  of a given state  $\omega_0^{(q)}$  on  $\mathcal{A}_0^{(q)}$  to  $\mathcal{A}_1^N$  may not converge to a state  $\omega_0^{(c)}$  on  $\mathcal{A}_0^{(c)}$  for  $N \rightarrow \infty$ .<sup>268</sup> States  $\omega_0^{(q)}$  on  $\bigcup_{N \in \mathbb{N}} \mathcal{A}_1^N$  that do have this property will here be called *classical*. In other words,  $\omega_{0|1/N}^{(q)}$  is classical when there exists a probability measure  $\mu_0$  on  $\mathcal{S}(\mathcal{A}_1)$  such that

$$(17) \quad \lim_{N \rightarrow \infty} \int_{\mathcal{S}(\mathcal{A}_1)} d\mu_0(\rho) (\rho^N(A_N) - \omega_{0|1/N}^{(q)}(A_N)) = 0$$

for each (approximately) symmetric sequence  $(A_1, A_2, \dots)$ . To analyze this notion we need a brief intermezzo on general  $C^*$ -algebras and their representations.

- A *folium* in the state space  $\mathcal{S}(\mathcal{B})$  of a  $C^*$ -algebra  $\mathcal{B}$  is a convex, norm-closed subspace  $\mathcal{F}$  of  $\mathcal{S}(\mathcal{B})$  with the property that if  $\omega \in \mathcal{F}$  and  $B \in \mathcal{B}$  such that  $\omega(B^*B) > 0$ , then the “reduced” state  $\omega_B : A \mapsto \omega(B^*AB)/\omega(B^*B)$  must be in  $\mathcal{F}$  [Haag *et al.*, 1970].<sup>269</sup> For example, if  $\pi$  is a representation of  $\mathcal{B}$  on a Hilbert space  $\mathcal{H}$ , then the set of all density matrices on  $\mathcal{H}$  (i.e. the  $\pi$ -normal states on  $\mathcal{B}$ )<sup>270</sup> comprises a folium  $\mathcal{F}_\pi$ . In particular, each state  $\omega$  on  $\mathcal{B}$  defines a folium  $\mathcal{F}_\omega \equiv \mathcal{F}_{\pi_\omega}$  through its GNS-representation  $\pi_\omega$ .
- Two representations  $\pi$  and  $\pi'$  are called *disjoint*, written  $\pi \perp \pi'$ , if no subrepresentation of  $\pi$  is (unitarily) equivalent to a subrepresentation of  $\pi'$  and

<sup>267</sup>For any fixed quasilocal sequence  $(A_1, A_2, \dots)$  and  $\varepsilon > 0$ , there is an  $N_\varepsilon$  such that  $|\omega_{1/N}(A_N) - \omega_{0|1/N}^{(q)}(A_N)| < \varepsilon$  for all  $N > N_\varepsilon$ .

<sup>268</sup>See footnote 288 below for an example

<sup>269</sup>See also [Haag, 1992]. The name ‘folium’ is very badly chosen, since  $\mathcal{S}(\mathcal{B})$  is by no means foliated by its folia; for example, a folium may contain subfolia.

<sup>270</sup>A state  $\omega$  on  $\mathcal{B}$  is called  $\pi$ -normal when it is of the form  $\omega(B) = \text{Tr } \rho \pi(B)$  for some density matrix  $\rho$ . Hence the  $\pi$ -normal states are the normal states on the von Neumann algebra  $\pi(\mathcal{B})''$ .

vice versa. They are said to be *quasi-equivalent*, written  $\pi \sim \pi'$ , when  $\pi$  has no subrepresentation disjoint from  $\pi'$ , and vice versa.<sup>271</sup> Quasi-equivalence is an equivalence relation  $\sim$  on the set of representations. See [Kadison and Ringrose, 1986, Ch. 10].

- Similarly, two states  $\rho, \sigma$  are called either quasi-equivalent ( $\rho \sim \sigma$ ) or disjoint ( $\rho \perp \sigma$ ) when the corresponding GNS-representations have these properties.
- A state  $\omega$  is called *primary* when the corresponding von Neumann algebra  $\pi_\omega(\mathcal{B})''$  is a factor.<sup>272</sup> Equivalently,  $\omega$  is primary iff each subrepresentation of  $\pi_\omega(\mathcal{B})$  is quasi-equivalent to  $\pi_\omega(\mathcal{B})$ , which is the case iff  $\pi_\omega(\mathcal{B})$  admits no (nontrivial) decomposition as the direct sum of two disjoint subrepresentations.

Now, there is a bijective correspondence between folia in  $\mathcal{S}(\mathcal{B})$  and quasi-equivalence classes of representations of  $\mathcal{B}$ , in that  $\mathcal{F}_\pi = \mathcal{F}_{\pi'}$  iff  $\pi \sim \pi'$ . Furthermore (as one sees from the GNS-construction), any folium  $\mathcal{F} \subset \mathcal{S}(\mathcal{B})$  is of the form  $\mathcal{F} = \mathcal{F}_\pi$  for some representation  $\pi(\mathcal{B})$ . Note that if  $\pi$  is injective (i.e. faithful), then the corresponding folium is dense in  $\mathcal{S}(\mathcal{B})$  in the weak\*-topology by Fell's Theorem. So in case that  $\mathcal{B}$  is simple,<sup>273</sup> any folium is weak\*-dense in the state space.

Two states need not be either disjoint or quasi-equivalent. This dichotomy does apply, however, within the class of primary states. Hence *two primary states are either disjoint or quasi-equivalent*. If  $\omega$  is primary, then each state in the folium of  $\pi_\omega$  is primary as well, and is quasi-equivalent to  $\omega$ . If, on the other hand,  $\rho$  and  $\sigma$  are primary and disjoint, then  $\mathcal{F}_\rho \cap \mathcal{F}_\sigma = \emptyset$ . Pure states are, of course, primary.<sup>274</sup> Furthermore, in thermodynamics pure phases are described by primary KMS states [Emch and Knops, 1970; Bratteli and Robinson, 1981; Haag, 1992; Sewell, 2002]. This apparent relationship between primary states and “purity” of some sort is confirmed by our description of macroscopic observables:<sup>275</sup>

- If  $\omega_0^{(q)}$  is a classical primary state on  $\mathcal{A}_0^{(q)} = \overline{\cup_{N \in \mathbb{N}} \mathcal{A}_1^N}$ , then the corresponding limit state  $\omega_0^{(c)}$  on  $\mathcal{A}_0^{(c)} = C(\mathcal{S}(\mathcal{A}_1))$  is pure (and hence given by a point in  $\mathcal{S}(\mathcal{A}_1)$ ).

<sup>271</sup>Equivalently, two representations  $\pi$  and  $\pi'$  are disjoint iff no  $\pi$ -normal state is  $\pi'$ -normal and vice versa, and quasi-equivalent iff each  $\pi$ -normal state is  $\pi'$ -normal and vice versa.

<sup>272</sup>A von Neumann algebra  $\mathcal{M}$  acting on a Hilbert space is called a *factor* when its center  $\mathcal{M} \cap \mathcal{M}'$  is trivial, i.e. consists of multiples of the identity.

<sup>273</sup>In the sense that it has no *closed* two-sided ideals. For example, the matrix algebra  $M_n(\mathbb{C})$  is simple for any  $n$ , as is its infinite-dimensional analogue, the  $C^*$ -algebra of all compact operators on a Hilbert space. The  $C^*$ -algebra of quasilocal observables of an infinite quantum systems is typically simple as well.

<sup>274</sup>Since the corresponding GNS-representation  $\pi_\omega$  is irreducible,  $\pi_\omega(\mathcal{B})'' = \mathcal{B}(\mathcal{H}_\omega)$  is a factor.

<sup>275</sup>These claims easily follow from Sewell [2002], §2.6.5, which in turn relies on Hepp [1972].

- If  $\rho_0^{(q)}$  and  $\sigma_0^{(q)}$  are classical primary states on  $\mathcal{A}_0^{(q)}$ , then

$$(18) \quad \rho_0^{(c)} = \sigma_0^{(c)} \Leftrightarrow \rho_0^{(q)} \sim \sigma_0^{(q)};$$

$$(19) \quad \rho_0^{(c)} \neq \sigma_0^{(c)} \Leftrightarrow \rho_0^{(q)} \perp \sigma_0^{(q)}.$$

As in (17), a general classical state  $\omega_0^{(q)}$  with limit state  $\omega_0^{(c)}$  on  $C(\mathcal{S}(\mathcal{A}_1))$  defines a probability measure  $\mu_0$  on  $\mathcal{S}(\mathcal{A}_1)$  by

$$(20) \quad \omega_0^{(c)}(f) = \int_{\mathcal{S}(\mathcal{A}_1)} d\mu_0 f,$$

which describes the probability distribution of the macroscopic observables in that state. As we have seen, this distribution is a delta function for primary states. In any case, it is insensitive to the microscopic details of  $\omega_0^{(q)}$  in the sense that local modifications of  $\omega_0^{(q)}$  do not affect the limit state  $\omega_0^{(c)}$  [Sewell, 2002]. Namely, it easily follows from (8) and the fact that the GNS-representation is cyclic that one can strengthen the second claim above:

*Each state in the folium  $\mathcal{F}_{\omega_0^{(q)}}$  of a classical state  $\omega_0^{(q)}$  is automatically classical and has the same limit state on  $\mathcal{A}_0^{(c)}$  as  $\omega_0^{(q)}$ .*

To make this discussion a bit more concrete, we now identify an important class of classical states on  $\overline{\cup_{N \in \mathbb{N}} \mathcal{A}_1^N}$ . We say that a state  $\omega$  on this  $C^*$ -algebra is *permutation-invariant* when each of its restrictions to  $\mathcal{A}_1^N$  is invariant under the natural action of the symmetric group  $\mathfrak{S}_N$  on  $\mathcal{A}_1^N$  (i.e.  $\sigma \in \mathfrak{S}_N$  maps an elementary tensor  $A_N = B_1 \otimes \cdots \otimes B_N \in \mathcal{A}_1^N$  to  $B_{\sigma(1)} \otimes \cdots \otimes B_{\sigma(N)}$ , cf. (5)). The structure of the set  $\mathcal{S}^\mathfrak{S}$  of all permutation-invariant states in  $\mathcal{S}(\mathcal{A}_0^{(q)})$  has been analyzed by Størmer [1969]. Like any compact convex set, it is the (weak\*-closed) convex hull of its extreme boundary  $\partial_e \mathcal{S}^\mathfrak{S}$ . The latter consists of all infinite product states  $\omega = \rho^\infty$ , where  $\rho \in \mathcal{S}(\mathcal{A}_1)$ . I.e. if  $A_0 \in \mathcal{A}_0^{(q)}$  is an equivalence class  $[A_1, A_2, \dots]$ , then

$$(21) \quad \rho^\infty(A_0) = \lim_{N \rightarrow \infty} \rho^N(A_N);$$

cf. (11). Equivalently, the restriction of  $\omega$  to any  $\mathcal{A}_1^N \subset \mathcal{A}_0^{(q)}$  is given by  $\otimes^N \rho$ . Hence  $\partial_e \mathcal{S}^\mathfrak{S}$  is isomorphic (as a compact convex set) to  $\mathcal{S}(\mathcal{A}_1)$  in the obvious way, and the primary states in  $\mathcal{S}^\mathfrak{S}$  are precisely the elements of  $\partial_e \mathcal{S}^\mathfrak{S}$ .

A general state  $\omega_0^{(q)}$  in  $\mathcal{S}^\mathfrak{S}$  has a unique decomposition<sup>276</sup>

$$(22) \quad \omega_0^{(q)}(A_0) = \int_{\mathcal{S}(\mathcal{A}_1)} d\mu(\rho) \rho^\infty(A_0),$$

where  $\mu$  is a probability measure on  $\mathcal{S}(\mathcal{A}_1)$  and  $A_0 \in \mathcal{A}_0^{(q)}$ .<sup>277</sup> The following beautiful illustration of the abstract theory [Unnerstall, 1990a,b] is then clear from (17) and (22):

*If  $\omega_0^{(q)}$  is permutation-invariant, then it is classical. The associated limit state  $\omega_0^{(c)}$  on  $\mathcal{A}_0^{(c)}$  is characterized by the fact that the measure  $\mu_0$  in (20) coincides with the measure  $\mu$  in (22).*<sup>278</sup>

### 6.3 Superselection rules

Infinite quantum systems are often associated with the notion of a superselection rule (or sector), which was originally introduced by Wick, Wightman and Wigner [1952] in the setting of standard quantum mechanics on a Hilbert space  $\mathcal{H}$ . The basic idea may be illustrated in the example of the boson/fermion (or “univalence”) superselection rule.<sup>279</sup> Here one has a *projective* unitary representation  $\mathcal{D}$  of the rotation group  $SO(3)$  on  $\mathcal{H}$ , for which  $\mathcal{D}(R_{2\pi}) = \pm 1$  for any rotation  $R_{2\pi}$  of  $2\pi$  around some axis. Specifically, on bosonic states  $\Psi_B$  one has  $\mathcal{D}(R_{2\pi})\Psi_B = \Psi_B$ , whereas on fermionic states  $\Psi_F$  the rule is  $\mathcal{D}(R_{2\pi})\Psi_F = -\Psi_F$ . Now the argument is that a rotation of  $2\pi$  accomplishes nothing, so that it cannot change the physical state of the system. This requirement evidently holds on the subspace  $\mathcal{H}_B \subset \mathcal{H}$  of bosonic states in  $\mathcal{H}$ , but it is equally well satisfied on the subspace  $\mathcal{H}_F \subset \mathcal{H}$  of fermionic states, since  $\Psi$  and  $z\Psi$  with  $|z| = 1$  describe the same physical state. However, if  $\Psi = c_B\Psi_B + c_F\Psi_F$  (with  $|c_B|^2 + |c_F|^2 = 1$ ), then  $\mathcal{D}(R_{2\pi})\Psi = c_B\Psi_B - c_F\Psi_F$ , which is not proportional to  $\Psi$  and apparently describes a genuinely different physical state from  $\Psi$ .

The way out is to deny this conclusion by declaring that  $\mathcal{D}(R_{2\pi})\Psi$  and  $\Psi$  *do* describe the same physical state, and this is achieved by postulating that no phys-

<sup>276</sup>This follows because  $\mathcal{S}^\mathfrak{S}$  is a so-called Bauer simplex [Alfsen, 1970]. This is a compact convex set  $K$  whose extreme boundary  $\partial_e K$  is closed and for which every  $\omega \in K$  has a *unique* decomposition as a probability measure supported by  $\partial_e K$ , in the sense that  $a(\omega) = \int_{\partial_e K} d\mu(\rho) a(\rho)$  for any continuous affine function  $a$  on  $K$ . For a unital  $C^*$ -algebra  $\mathcal{A}$  the continuous affine functions on the state space  $K = \mathcal{S}(\mathcal{A})$  are precisely the elements  $A$  of  $\mathcal{A}$ , reinterpreted as functions  $\hat{A}$  on  $\mathcal{S}(\mathcal{A})$  by  $\hat{A}(\omega) = \omega(A)$ . For example, the state space  $\mathcal{S}(\mathcal{A})$  of a commutative unital  $C^*$ -algebra  $\mathcal{A}$  is a Bauer simplex, which consists of all (regular Borel) probability measures on the pre state space  $\mathcal{P}(\mathcal{A})$ .

<sup>277</sup>This is a quantum analogue of De Finetti’s representation theorem in classical probability theory [Heath and Sudderth, 1976; van Fraassen, 1991]; see also [Hudson and Moody, 1975/76] and [Caves *et al.*, 2002].

<sup>278</sup>In fact, each state in the folium  $\mathcal{F}^\mathfrak{S}$  in  $\mathcal{S}(\mathcal{A}_0^{(q)})$  corresponding to the (quasi-equivalence class of) the representation  $\oplus_{[\omega \in \mathcal{S}^\mathfrak{S}]} \pi_\omega$  is classical.

<sup>279</sup>See also [Giulini, 2003] for a modern mathematical treatment.

ical *observables*  $A$  (in their usual mathematical guise as operators on  $\mathcal{H}$ ) exist for which  $(\Psi_B, A\Psi_F) \neq 0$ . For in that case one has

$$(23) \quad (c_B\Psi_B \pm c_F\Psi_F, A(c_B\Psi_B \pm c_F\Psi_F)) = |c_B|^2(\Psi_B, A\Psi_B) + |c_F|^2(\Psi_F, A\Psi_F)$$

for any *observable*  $A$ , so that  $(\mathcal{D}(R_{2\pi})\Psi, A\mathcal{D}(R_{2\pi})\Psi) = (\Psi, A\Psi)$  for any  $\Psi \in \mathcal{H}$ . Since any quantum-mechanical prediction ultimately rests on expectation values  $(\Psi, A\Psi)$  for physical observables  $A$ , the conclusion is that a rotation of  $2\pi$  indeed does nothing to the system. This is codified by saying that superpositions of the type  $c_B\Psi_B + c_F\Psi_F$  are *incoherent* (whereas superpositions  $c_1\Psi_1 + c_2\Psi_2$  with  $\Psi_1, \Psi_2$  both in either  $\mathcal{H}_B$  or in  $\mathcal{H}_F$  are *coherent*). Each of the subspaces  $\mathcal{H}_B$  and  $\mathcal{H}_F$  of  $\mathcal{H}$  is said to be a *superselection sector*, and the statement that  $(\Psi_B, A\Psi_F) = 0$  for any observable  $A$  and  $\Psi_B \in \mathcal{H}_B$  and  $\Psi_F \in \mathcal{H}_F$  is called a *superselection rule*.<sup>280</sup>

The price one pays for this solution is that states of the form  $c_B\Psi_B + c_F\Psi_F$  with  $c_B \neq 0$  and  $c_F \neq 0$  are mixed, as one sees from (23). More generally, if  $\mathcal{H} = \oplus_{\lambda \in \Lambda} \mathcal{H}_\lambda$  with  $(\Psi, A\Phi) = 0$  whenever  $A$  is an observable,  $\Psi \in \mathcal{H}_\lambda$ ,  $\Phi \in \mathcal{H}_{\lambda'}$ , and  $\lambda \neq \lambda'$ , and if in addition for each  $\lambda$  and each pair  $\Psi, \Phi \in \mathcal{H}_\lambda$  there exists an observable  $A$  for which  $(\Psi, A\Phi) \neq 0$ , then the subspaces  $\mathcal{H}_\lambda$  are called superselection sectors in  $\mathcal{H}$ . Again a key consequence of the occurrence of superselection sectors is that unit vectors of the type  $\Psi = \sum_\lambda c_\lambda \Psi_\lambda$  with  $\Psi \in \mathcal{H}_\lambda$  (and  $c_\lambda \neq 0$  for at least two  $\lambda$ 's) define mixed states

$$\psi(A) = (\Psi, A\Psi) = \sum_\lambda |c_\lambda|^2 (\Psi_\lambda, A\Psi_\lambda) = \sum_\lambda |c_\lambda|^2 \psi_\lambda(A).$$

This procedure is rather ad hoc. A much deeper approach to superselection theory was developed by Haag and collaborators; see [Roberts and Roepstorff, 1969] for an introduction. Here the starting point is the abstract  $C^*$ -algebra of observables  $\mathcal{A}$  of a given quantum system, and superselection sectors are reinterpreted as equivalence classes (under unitary isomorphism) of irreducible representations of  $\mathcal{A}$  (satisfying a certain selection criterion — see below). The connection between the concrete Hilbert space approach to superselection sectors discussed above and the abstract  $C^*$ -algebraic approach is given by the following lemma [Hepp, 1972]:<sup>281</sup>

*Two pure states  $\rho, \sigma$  on a  $C^*$ -algebra  $\mathcal{A}$  define different sectors iff for each representation  $\pi(\mathcal{A})$  on a Hilbert space  $\mathcal{H}$  containing unit vectors  $\Psi_\rho, \Psi_\sigma$  such that  $\rho(A) = (\Psi_\rho, \pi(A)\Psi_\rho)$  and  $\sigma(A) = (\Psi_\sigma, \pi(A)\Psi_\sigma)$  for all  $A \in \mathcal{A}$ , one has  $(\Psi_\rho, \pi(A)\Psi_\sigma) = 0$  for all  $A \in \mathcal{A}$ .*

In practice, however, most irreducible representations of a typical  $C^*$ -algebra  $\mathcal{A}$  used in physics are physically irrelevant mathematical artefacts. Such representations may be excluded from consideration by some *selection criterion*. What this

<sup>280</sup>In an ordinary selection rule between  $\Psi$  and  $\Phi$  one merely has  $(\Psi, H\Phi) = 0$  for the Hamiltonian  $H$ .

<sup>281</sup>Hepp proved a more general version of this lemma, in which ‘Two pure states  $\rho, \sigma$  on a  $C^*$ -algebra  $\mathcal{B}$  define different sectors iff. . .’ is replaced by ‘Two states  $\rho, \sigma$  on a  $C^*$ -algebra  $\mathcal{B}$  are disjoint iff. . .’

means depends on the context. For example, in quantum field theory this notion is made precise in the so-called DHR theory (reviewed by Roberts [1990], Haag [1992], Araki [1999], and Halvorson [2005]). In the class of theories discussed in the preceding two subsections, we take the algebra of observables  $\mathcal{A}$  to be  $\mathcal{A}_0^{(q)}$  — essentially for reasons of human limitation — and for pedagogical reasons define (equivalence classes of) irreducible representations of  $\mathcal{A}_0^{(q)}$  as superselection sectors, henceforth often just called *sectors*, only when they are equivalent to the GNS-representation given by a permutation-invariant pure state on  $\mathcal{A}_0^{(q)}$ . In particular, such a state is classical. On this selection criterion, the results in the preceding subsection trivially imply that there is a bijective correspondence between pure states on  $\mathcal{A}_1$  and sectors of  $\mathcal{A}_0^{(q)}$ . The sectors of the commutative  $C^*$ -algebra  $\mathcal{A}_0^{(c)}$  are just the points of  $\mathcal{S}(\mathcal{A}_1)$ ; note that a *mixed* state on  $\mathcal{A}_1$  defines a *pure* state on  $\mathcal{A}_0^{(c)}$ ! The role of the sectors of  $\mathcal{A}_1$  in connection with those of  $\mathcal{A}_0^{(c)}$  will be clarified in Subsection 6.5.

Whatever the model or the selection criterion, it is enlightening (and to some extent even in accordance with experimental practice) to consider superselection sectors entirely from the perspective of the pure states on the algebra of observables  $\mathcal{A}$ , removing  $\mathcal{A}$  itself and its representations from the scene. To do so, we equip the space  $\mathcal{P}(\mathcal{A})$  of pure states on  $\mathcal{A}$  with the structure of a transition probability space [von Neumann, 1981; Mielnik, 1968].<sup>282</sup> A *transition probability* on a set  $\mathcal{P}$  is a function

$$(24) \quad p : \mathcal{P} \times \mathcal{P} \rightarrow [0, 1]$$

that satisfies

$$(25) \quad p(\rho, \sigma) = 1 \iff \rho = \sigma$$

and

$$(26) \quad p(\rho, \sigma) = 0 \iff p(\sigma, \rho) = 0.$$

A set with such a transition probability is called a *transition probability space*. Now, the pure state space  $\mathcal{P}(\mathcal{A})$  of a  $C^*$ -algebra  $\mathcal{A}$  carries precisely this structure if we define<sup>283</sup>

$$(27) \quad p(\rho, \sigma) := \inf\{\rho(A) \mid A \in \mathcal{A}, 0 \leq A \leq 1, \sigma(A) = 1\}.$$

To give a more palatable formula, note that since pure states are primary, two pure states  $\rho, \sigma$  are either disjoint ( $\rho \perp \sigma$ ) or else (quasi, hence unitarily) equivalent ( $\rho \sim \sigma$ ). In the first case, (27) yields

$$(28) \quad p(\rho, \sigma) = 0 \quad (\rho \perp \sigma).$$

<sup>282</sup>See also [Beltrametti and Cassinelli, 1984] or [Landsman, 1998] for concise reviews.

<sup>283</sup>This definition applies to the case that  $\mathcal{A}$  is unital; see [Landsman, 1998] for the general case. An analogous formula defines a transition probability on the extreme boundary of any compact convex set.

In the second case it follows from Kadison's transitivity theorem (cf. Thm. 10.2.6 in [Kadison and Ringrose, 1986]) that the Hilbert space  $\mathcal{H}_\rho$  from the GNS-representation  $\pi_\rho(\mathcal{A})$  defined by  $\rho$  contains a unit vector  $\Omega_\sigma$  (unique up to a phase) such that

$$(29) \quad \sigma(A) = (\Omega_\sigma, \pi_\rho(A)\Omega_\sigma).$$

Eq. (27) then leads to the well-known expression

$$(30) \quad p(\rho, \sigma) = |(\Omega_\rho, \Omega_\sigma)|^2 \quad (\rho \sim \sigma).$$

In particular, if  $\mathcal{A}$  is commutative, then

$$(31) \quad p(\rho, \sigma) = \delta_{\rho\sigma}.$$

For  $\mathcal{A} = M_2(\mathbb{C})$  one obtains

$$(32) \quad p(\rho, \sigma) = \frac{1}{2}(1 + \cos \theta_{\rho\sigma}),$$

where  $\theta_{\rho\sigma}$  is the angular distance between  $\rho$  and  $\sigma$  (seen as points on the two-sphere  $S^2 = \partial_e B^3$ , cf. (3) etc.), measured along a great circle.

Superselection sectors may now be defined for any transition probability spaces  $\mathcal{P}$ . A family of subsets of  $\mathcal{P}$  is called *orthogonal* if  $p(\rho, \sigma) = 0$  whenever  $\rho$  and  $\sigma$  do not lie in the same subset. The space  $\mathcal{P}$  is called *reducible* if it is the union of two (nonempty) orthogonal subsets; if not, it is said to be *irreducible*. A *component* of  $\mathcal{P}$  is a subset  $\mathcal{C} \subset \mathcal{P}$  such that  $\mathcal{C}$  and  $\mathcal{P} \setminus \mathcal{C}$  are orthogonal. An irreducible component of  $\mathcal{P}$  is called a (*superselection*) *sector*. Thus  $\mathcal{P}$  is the disjoint union of its sectors. For  $\mathcal{P} = \mathcal{P}(\mathcal{A})$  this reproduces the algebraic definition of a superselection sector (modulo the selection criterion) via the correspondence between states and representations given by the GNS-constructions. For example, in the commutative case  $\mathcal{A} \cong C(X)$  each point in  $X \cong \mathcal{P}(\mathcal{A})$  is its own little sector.

#### 6.4 A simple example: the infinite spin chain

Let us illustrate the occurrence of superselection sectors in a simple example, where the algebra of observables is  $\mathcal{A}_0^{(q)}$  with  $\mathcal{A}_1 = M_2(\mathbb{C})$ . Let  $\mathcal{H}_1 = \mathbb{C}^2$ , so that  $\mathcal{H}_1^N = \otimes^N \mathbb{C}^2$  is the tensor product of  $N$  copies of  $\mathbb{C}^2$ . It is clear that  $\mathcal{A}_1^N$  acts on  $\mathcal{H}_1^N$  in a natural way (i.e. componentwise). This defines an irreducible representation  $\pi_N$  of  $\mathcal{A}_1^N$ , which is indeed its unique irreducible representation (up to unitary equivalence). In particular, for  $N < \infty$  the quantum system whose algebra of observables is  $\mathcal{A}_1^N$  (such as a chain with  $N$  two-level systems) has no superselection rules. We define the  $N \rightarrow \infty$  limit " $(M_2(\mathbb{C}))^\infty$ " of the  $C^*$ -algebras  $(M_2(\mathbb{C}))^N$  as the inductive limit  $\mathcal{A}_0^{(q)}$  for  $\mathcal{A}_1 = M_2(\mathbb{C})$ , as introduced in Subsection 6.2; see (13). The definition of " $\otimes^\infty \mathbb{C}^2$ " is slightly more involved, as follows [von Neumann, 1938].

For any Hilbert space  $\mathcal{H}_1$ , let  $\Psi$  be a sequence  $(\Psi_1, \Psi_2, \dots)$  with  $\Psi_n \in \mathcal{H}_1$ . The space  $\mathbf{H}_1$  of such sequences is a vector space in the obvious way. Now let  $\Psi$  and  $\Phi$  be two such sequences, and write  $(\Psi_n, \Phi_n) = \exp(i\alpha_n)|(\Psi_n, \Phi_n)|$ . If  $\sum_n |\alpha_n| = \infty$ ,



we define the (pre-) inner product  $(\Psi, \Phi)$  to be zero. If  $\sum_n |\alpha_n| < \infty$ , we put  $(\Psi, \Phi) = \prod_n (\Psi_n, \Phi_n)$  (which, of course, may still be zero!). The (vector space) quotient of  $\mathcal{H}_1$  by the space of sequences  $\Psi$  for which  $(\Psi, \Psi) = 0$  can be completed to a Hilbert space  $\mathcal{H}_1^\infty$  in the induced inner product, called the *complete* infinite tensor product of the Hilbert space  $\mathcal{H}_1$  (over the index set  $\mathbb{N}$ ).<sup>284</sup> We apply this construction with  $\mathcal{H}_1 = \mathbb{C}^2$ . If  $(e_i)$  is some basis of  $\mathbb{C}^2$ , an orthonormal basis of  $\mathcal{H}_1^\infty$  then consists of all different infinite strings  $e_{i_1} \otimes \cdots e_{i_n} \otimes \cdots$ , where  $e_{i_n}$  is  $e_i$  regarded as a vector in  $\mathbb{C}^2$ .<sup>285</sup> We denote the multi-index  $(i_1, \dots, i_n, \dots)$  simply by  $I$ , and the corresponding basis vector by  $e_I$ .

This Hilbert space  $\mathcal{H}_1^\infty$  carries a natural faithful representation  $\pi$  of  $\mathcal{A}_0^{(q)}$ : if  $A_0 \in \mathcal{A}_0^{(q)}$  is an equivalence class  $[A_1, A_2, \dots]$ , then  $\pi(A_0)e_I = \lim_{N \rightarrow \infty} A_N e_i$ , where  $A_N$  acts on the first  $N$  components of  $e_I$  and leaves the remainder unchanged.<sup>286</sup> Now the point is that although each  $\mathcal{A}_1^N$  acts irreducibly on  $\mathcal{H}_1^N$ , the representation  $\pi(\mathcal{A}_0^{(q)})$  on  $\mathcal{H}_1^\infty$  thus constructed is highly reducible. The reason for this is that by definition (quasi-) local elements of  $\mathcal{A}_0^{(q)}$  leave the infinite tail of a vector in  $\mathcal{H}_1^\infty$  (almost) unaffected, so that vectors with different tails lie in different superselection sectors. Without the quasi-locality condition on the elements of  $\mathcal{A}_0^{(q)}$ , no superselection rules would arise. For example, in terms of the usual basis

$$(33) \quad \left\{ \uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$$

of  $\mathbb{C}^2$ , the vectors  $\Psi_\uparrow = \uparrow \otimes \uparrow \cdots \uparrow \cdots$  (i.e. an infinite product of ‘up’ vectors) and  $\Psi_\downarrow = \downarrow \otimes \downarrow \cdots \downarrow \cdots$  (i.e. an infinite product of ‘down’ vectors) lie in different sectors. The reason why the inner product  $(\Psi_\uparrow, \pi(A)\Psi_\downarrow)$  vanishes for any  $A \in \mathcal{A}_0^{(q)}$  is that for local observables  $A$  one has  $\pi(A) = A_M \otimes 1 \otimes \cdots 1 \cdots$  for some  $A_M \in \mathcal{B}(\mathcal{H}_M)$ ; the inner product in question therefore involves infinitely many factors  $(\uparrow, 1 \downarrow) = (\uparrow, \downarrow) = 0$ . For quasilocal  $A$  the operator  $\pi(A)$  might have a small nontrivial tail, but the inner product vanishes nonetheless by an approximation argument.

More generally, elementary analysis shows that  $(\Psi_u, \pi(A)\Psi_v) = 0$  whenever  $\Psi_u = \otimes^\infty u$  and  $\Psi_v = \otimes^\infty v$  for unit vectors  $u, v \in \mathbb{C}^2$  with  $u \neq v$ . The corresponding vector states  $\psi_u$  and  $\psi_v$  on  $\mathcal{A}_0^{(q)}$  (i.e.  $\psi_u(A) = (\Psi_u, \pi(A)\Psi_u)$  etc.) are obviously permutation-invariant and hence classical. Identifying  $\mathcal{S}(M_2(\mathbb{C}))$  with  $B^3$ , as in (3), the corresponding limit state  $(\psi_u)_0$  on  $\mathcal{A}_0^{(c)}$  defined by  $\psi_u$  is given by (evaluation at) the point  $\tilde{u} = (x, y, z)$  of  $\partial_e B^3 = S^2$  (i.e. the two-sphere) for which the corresponding density matrix  $\rho(\tilde{u})$  is the projection operator onto  $u$ . It

<sup>284</sup>Each fixed  $\Psi \in \mathcal{H}_1$  defines an *incomplete* tensor product  $\mathcal{H}_\Psi^\infty$ , defined as the closed subspace of  $\mathcal{H}_1^\infty$  consisting of all  $\Phi$  for which  $\sum_n |(\Psi_n, \Phi_n) - 1| < \infty$ . If  $\mathcal{H}_1$  is separable, then so is  $\mathcal{H}_\Psi^\infty$  (in contrast to  $\mathcal{H}_1^\infty$ , which is an uncountable direct sum of the  $\mathcal{H}_\Psi^\infty$ ).

<sup>285</sup>The cardinality of the set of all such strings equals that of  $\mathbb{R}$ , so that  $\mathcal{H}_1^\infty$  is non-separable, as claimed.

<sup>286</sup>Indeed, this yields an alternative way of defining  $\overline{\cup_{N \in \mathbb{N}} \mathcal{A}_1^N}$  as the norm closure of the union of all  $\mathcal{A}_1^N$  acting on  $\mathcal{H}_1^\infty$  in the stated way.

follows that  $\psi_u$  and  $\psi_v$  are disjoint; cf. (19). We conclude that each unit vector  $u \in \mathbb{C}^2$  determines a superselection sector  $\pi_u$ , namely the GNS-representation of the corresponding state  $\psi_u$ , and that each such sector is realized as a subspace  $\mathcal{H}_u$  of  $\mathcal{H}_1^\infty$  (viz.  $\mathcal{H}_u = \pi(\mathcal{A}_0^{(q)})\Psi_u$ ). Moreover, since a permutation-invariant state on  $\mathcal{A}_0^{(q)}$  is pure iff it is of the form  $\psi_u$ , we have found all superselection sectors of our system. Thus in what follows we may concentrate our attention on the subspace (of  $\mathcal{H}_1^\infty$ ) and subrepresentation (of  $\pi$ )

$$(34) \quad \begin{aligned} \mathcal{H}_\mathfrak{S} &= \bigoplus_{\tilde{u} \in S^2} \mathcal{H}_u; \\ \pi_\mathfrak{S}(\mathcal{A}_0^{(q)}) &= \bigoplus_{\tilde{u} \in S^2} \pi_u(\mathcal{A}_0^{(q)}), \end{aligned}$$

where  $\pi_u$  is simply the restriction of  $\pi$  to  $\mathcal{H}_u \subset \mathcal{H}_1^\infty$ .

In the presence of superselection sectors one may construct operators that distinguish different sectors whilst being a multiple of the unit in each sector. In quantum field theory these are typically global charges, and in our example the macroscopic observables play this role. To see this, we return to Subsection 6.1. It is not difficult to show that for any approximately symmetric sequence  $(A_1, A_2, \dots)$  the limit

$$(35) \quad \bar{A} = \lim_{N \rightarrow \infty} \pi_\mathfrak{S}(A_N)$$

exists in the strong operator topology on  $\mathcal{B}(\mathcal{H}_\mathfrak{S})$  [Bona, 1988]. Moreover, if  $A_0 \in \mathcal{A}_0^{(c)} = C(\mathcal{S}(\mathcal{A}_1))$  is the function defined by the given sequence,<sup>287</sup> then the map  $A_0 \mapsto \bar{A}$  defines a faithful representation of  $\mathcal{A}_0^{(c)}$  on  $\mathcal{H}_\mathfrak{S}$ , which we call  $\pi_\mathfrak{S}$  as well (by abuse of notation). An easy calculation in fact shows that  $\pi_\mathfrak{S}(A_0)\Psi = A_0(\tilde{u})\Psi$  for  $\Psi \in \mathcal{H}_u$ , or, in other words,

$$(36) \quad \pi_\mathfrak{S}(A_0) = \bigoplus_{\tilde{u} \in S^2} A_0(\tilde{u})1_{\mathcal{H}_u}.$$

Thus the  $\pi_\mathfrak{S}(A_0)$  indeed serve as the operators in question.

To illustrate how delicate all this is, it may be interesting to note that even for symmetric sequences the limit  $\lim_{N \rightarrow \infty} \pi(A_N)$  does not exist on  $\mathcal{H}_1^\infty$ , not even in the strong topology.<sup>288</sup> On the positive side, it can be shown that  $\lim_{N \rightarrow \infty} \pi(A_N)\Psi$  exists as an element of the von Neumann algebra  $\pi(\mathcal{A}_0^{(q)})''$  whenever the vector state  $\psi$  defined by  $\Psi$  lies in the folium  $\mathcal{F}^\mathfrak{S}$  generated by all permutation-invariant states [Bona, 1988; Unnerstall, 1990a].

This observation is part of a general theory of macroscopic observables in the setting of von Neumann algebras [Primas, 1983; Rieckers, 1984; Amann, 1986; 1987; Morchio and Strocchi, 1987; Bona, 1988; 1989; Unnerstall, 1990a; 1990b; Breuer,

<sup>287</sup> Recall that  $A_0(\omega) = \lim_{N \rightarrow \infty} \omega^N(A_N)$ .

<sup>288</sup> For example, let us take the sequence  $A_N = j_{N1}(\text{diag}(1, -1))$  and the vector  $\Psi = \uparrow \downarrow \downarrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \dots$ , where a sequence of  $2^N$  factors of  $\uparrow$  is followed by  $2^{N+1}$  factors of  $\downarrow$ , etc. Then the sequence  $\{\pi(A_N)\Psi\}_{N \in \mathbb{N}}$  in  $\mathcal{H}_1^\infty$  diverges: the subsequence where  $N$  runs over all numbers  $2^n$  with  $n$  odd converges to  $\frac{1}{3}\Psi$ , whereas the subsequence where  $N$  runs over all  $2^n$  with  $n$  even converges to  $-\frac{1}{3}\Psi$ .

1994; Atmanspacher *et al.*, 1999], which complements the purely  $C^*$ -algebraic approach of Raggio and Werner [1989; 1991], Duffield and Werner [1992a,b,c], and Duffield *et al.* [1992] explained above.<sup>289</sup> In our opinion, the latter has the advantage that conceptually the passage to the limit  $N \rightarrow \infty$  (and thereby the idealization of a large system as an infinite one) is very satisfactory, especially in our reformulation in terms of continuous fields of  $C^*$ -algebras. Here the commutative  $C^*$ -algebra  $\mathcal{A}_0^{(c)}$  of macroscopic observables of the infinite system is glued to the noncommutative algebras  $\mathcal{A}_1^N$  of the corresponding finite systems in a continuous way, and the continuous sections of the ensuing continuous field of  $C^*$ -algebras  $\mathcal{A}^{(c)}$  exactly describe how *macroscopic* quantum observables of the finite systems converge to classical ones. *Microscopic* quantum observables of the pertinent finite systems, on the other hand, converge to quantum observables of the infinite quantum system, and this convergence is described by the continuous sections of the continuous field of  $C^*$ -algebras  $\mathcal{A}^{(q)}$ . This entirely avoids the language of superselection rules, which rather displays a shocking *discontinuity* between finite and infinite systems: for superselection rules do not exist in finite systems!<sup>290</sup>

### 6.5 Poisson structure and dynamics

We now pass to the discussion of time-evolution in infinite systems of the type considered so far. We start with the observation that the state space  $\mathcal{S}(\mathcal{B})$  of a finite-dimensional  $C^*$ -algebra  $\mathcal{B}$  (for simplicity assumed unital in what follows) is a Poisson manifold (cf. Subsection 4.3) in a natural way. A similar statement holds in the infinite-dimensional case, and we carry the reader through the necessary adaptations of the main argument by means of footnotes.<sup>291</sup> We write  $K = \mathcal{S}(\mathcal{B})$ .

<sup>289</sup>Realistic models have been studied in the context of both the  $C^*$ -algebraic and the von Neumann algebraic approach by Rieckers and his associates. See, for example, [Honegger and Rieckers, 1994; Gerisch *et al.*, 1999; Gerisch, *et al.* 2003], and many other papers. For altogether different approaches to macroscopic observables see [van Kampen, 1954; 1988; 1993; Wan and Fountain, 1998; Harrison and Wan, 1997; Wan *et al.*, 1998; Fröhlich *et al.*, 2002], and [Poulin, 2004].

<sup>290</sup>We here refer to superselection rules in the traditional sense of inequivalent irreducible representations of *simple*  $C^*$ -algebras. For topological reasons certain finite-dimensional systems are described by (non-simple)  $C^*$ -algebras that do admit inequivalent irreducible representations [Landsman, 1990a,b].

<sup>291</sup>Of which this is the first. When  $\mathcal{B}$  is infinite-dimensional, the state space  $\mathcal{S}(\mathcal{B})$  is no longer a manifold, let alone a Poisson manifold, but a *Poisson space* [Landsman, 1997; 1998]. This is a generalization of a Poisson manifold, which turns a crucial *property* of the latter into a *definition*. This property is the foliation of a Poisson manifold by its symplectic leaves [Weinstein, 1983], and the corresponding definition is as follows: A *Poisson space*  $P$  is a Hausdorff space of the form  $P = \cup_{\alpha} S_{\alpha}$  (disjoint union), where each  $S_{\alpha}$  is a symplectic manifold (possibly infinite-dimensional) and each injection  $\iota_{\alpha} : S_{\alpha} \hookrightarrow P$  is continuous. Furthermore, one has a linear subspace  $F \subset C(P, \mathbb{R})$  that separates points and has the property that the restriction of each  $f \in F$  to each  $S_{\alpha}$  is smooth. Finally, if  $f, g \in F$  then  $\{f, g\} \in F$ , where the Poisson bracket is defined by  $\{f, g\}(\iota_{\alpha}(\sigma)) = \{\iota_{\alpha}^* f, \iota_{\alpha}^* g\}_{\alpha}(\sigma)$ . Clearly, a Poisson manifold  $M$  defines a Poisson space if one takes  $P = M$ ,  $F = C^{\infty}(M)$ , and the  $S_{\alpha}$  to be the symplectic leaves defined by the given Poisson bracket. Thus we refer to the manifolds  $S_{\alpha}$  in the above definition as the *symplectic leaves* of  $P$  as well.

Firstly, an element  $A \in \mathcal{B}$  defines a linear function  $\hat{A}$  on  $\mathcal{B}^*$  and hence on  $K$  (namely by restriction) through  $\hat{A}(\omega) = \omega(A)$ . For such functions we define the Poisson bracket by

$$(37) \quad \{\hat{A}, \hat{B}\} = i\widehat{[A, B]}.$$

Here the factor  $i$  has been inserted in order to make the Poisson bracket of two real-valued functions real-valued again; for  $\hat{A}$  is real-valued on  $K$  precisely when  $A$  is self-adjoint, and if  $A^* = A$  and  $B^* = B$ , then  $i[A, B]$  is self-adjoint (whereas  $[A, B]$  is skew-adjoint). In general, for  $f, g \in C^\infty(K)$  we put

$$(38) \quad \{f, g\}(\omega) = i\omega([df_\omega, dg_\omega]),$$

interpreted as follows.<sup>292</sup> Let  $\mathcal{B}_\mathbb{R}$  be the self-adjoint part of  $\mathcal{B}$ , and interpret  $K$  as a subspace of  $\mathcal{B}_\mathbb{R}^*$ ; since a state  $\omega$  satisfies  $\omega(A^*) = \overline{\omega(A)}$  for all  $A \in \mathcal{B}$ , it is determined by its values on self-adjoint elements. Subsequently, we identify the tangent space at  $\omega$  with

$$(39) \quad T_\omega K = \{\rho \in \mathcal{B}_\mathbb{R}^* \mid \rho(1) = 0\} \subset \mathcal{B}_\mathbb{R}^*$$

and the cotangent space at  $\omega$  with the quotient (of real Banach spaces)

$$(40) \quad T_\omega^* K = \mathcal{B}_\mathbb{R}^{**} / \mathbb{R}1,$$

where the unit  $1 \in \mathcal{B}$  is regarded as an element of  $\mathcal{B}^{**}$  through the canonical embedding  $\mathcal{B} \subset \mathcal{B}^{**}$ . Consequently, the differential forms  $df$  and  $dg$  at  $\omega \in K$  define elements of  $\mathcal{B}_\mathbb{R}^{**} / \mathbb{R}1$ . The commutator in (38) is then defined as follows: one lifts  $df_\omega \in \mathcal{B}_\mathbb{R}^{**} / \mathbb{R}1$  to  $\mathcal{B}_\mathbb{R}^{**}$ , and uses the natural isomorphism  $\mathcal{B}^{**} \cong \mathcal{B}$  typical of finite-dimensional vector spaces.<sup>293</sup> The arbitrariness in this lift is a multiple of 1, which drops out of the commutator. Hence  $i[df_\omega, dg_\omega]$  is an element of  $\mathcal{B}_\mathbb{R}^{**} \cong \mathcal{B}_\mathbb{R}$ , on which the value of the functional  $\omega$  is defined.<sup>294</sup> This completes the definition of the Poisson bracket; one easily recovers (37) as a special case of (38).

The symplectic leaves of the given Poisson structure on  $K$  have been determined by Duffield and Werner [1992a].<sup>295</sup> Namely:

*Two states  $\rho$  and  $\sigma$  lie in the same symplectic leaf of  $\mathcal{S}(\mathcal{B})$  iff  $\rho(A) = \sigma(UAU^*)$  for some unitary  $U \in \mathcal{B}$ .*

<sup>292</sup>In the infinite-dimensional case  $C^\infty(K)$  is defined as the intersection of the smooth functions on  $K$  with respect to its Banach manifold structure and the space  $C(K)$  of weak\*-continuous functions on  $K$ . The differential forms  $df$  and  $dg$  in (38) also require an appropriate definition; see [Duffield and Werner, 1992a; Bona, 2000], and [Odzijewicz and Ratiu, 2003] for the technicalities.

<sup>293</sup>In the infinite-dimensional case one uses the canonical identification between  $\mathcal{B}^{**}$  and the enveloping von Neumann algebra of  $\mathcal{B}$  to define the commutator.

<sup>294</sup>If  $\mathcal{B}$  is infinite-dimensional, one here regards  $\mathcal{B}^*$  as the predual of the von Neumann algebra  $\mathcal{B}^{**}$ .

<sup>295</sup>See also [Bona, 2000] for the infinite-dimensional special case where  $\mathcal{B}$  is the  $C^*$ -algebra of compact operators.

When  $\rho$  and  $\sigma$  are pure, this is the case iff the corresponding GNS-representations  $\pi_\rho(\mathcal{B})$  and  $\pi_\sigma(\mathcal{B})$  are unitarily equivalent,<sup>296</sup> but in general the implication holds only in one direction: if  $\rho$  and  $\sigma$  lie in the same leaf, then they have unitarily equivalent GNS-representations.<sup>297</sup>

It follows from this characterization of the symplectic leaves of  $K = \mathcal{S}(\mathcal{B})$  that the pure state space  $\partial_e K = \mathcal{P}(\mathcal{B})$  inherits the Poisson bracket from  $K$ , and thereby becomes a Poisson manifold in its own right.<sup>298</sup> This leads to an important connection between the superselection sectors of  $\mathcal{B}$  and the Poisson structure on  $\mathcal{P}(\mathcal{B})$  [Landsman, 1997; 1998]:

*The sectors of the pure state space  $\mathcal{P}(\mathcal{B})$  of a  $C^*$ -algebra  $\mathcal{B}$  as a transition probability space coincide with its symplectic leaves as a Poisson manifold.*

For example, when  $\mathcal{B} \cong C(X)$  is commutative, the space  $\mathcal{S}(C(X))$  of all (regular Borel) probability measures on  $X$  acquires a Poisson bracket that is identically zero, as does its extreme boundary  $X$ . It follows from (31) that the sectors in  $X$  are its points, and so are its symplectic leaves (in view of their definition and the vanishing Poisson bracket). The simplest noncommutative case is  $\mathcal{B} = M_2(\mathbb{C})$ , for which the symplectic leaves of the state space  $K = \mathcal{S}(M_2(\mathbb{C})) \cong B^3$  (cf. (3)) are the spheres with constant radius.<sup>299</sup> The sphere with radius 1 consists of points in  $B^3$  that correspond to pure states on  $M_2(\mathbb{C})$ , all interior symplectic leaves of  $K$  coming from mixed states on  $M_2(\mathbb{C})$ .

The coincidence of sectors and symplectic leaves of  $\mathcal{P}(\mathcal{B})$  is a compatibility condition between the transition probability structure and the Poisson structure. It is typical of the specific choices (27) and (38), respectively, and hence of quantum theory. In classical mechanics one has the freedom of equipping a manifold  $M$  with an arbitrary Poisson structure, and yet use  $C_0(M)$  as the commutative  $C^*$ -algebra of observables. The transition probability (31) (which follows from (27) in the commutative case) are clearly the correct ones in classical physics, but since the

<sup>296</sup>Cf. Thm. 10.2.6 in [Kadison and Ringrose, 1986].

<sup>297</sup>An important step of the proof is the observation that the Hamiltonian vector field  $\xi_f(\omega) \in T_\omega K \subset \mathcal{A}_\mathbb{R}^*$  of  $f \in C^\infty(K)$  is given by  $\langle \xi_f(\omega), B \rangle = i[df_\omega, B]$ , where  $B \in \mathcal{B}_\mathbb{R} \subset \mathcal{B}_\mathbb{R}^{**}$  and  $df_\omega \in \mathcal{B}_\mathbb{R}^{**}/\mathbb{R}1$ . (For example, this gives  $\xi_{\hat{A}} \hat{B} = i[\widehat{A}, \widehat{B}] = \{\hat{A}, \hat{B}\}$  by (37), as it should be.) If  $\varphi_t^h$  denotes the Hamiltonian flow of  $h$  at time  $t$ , it follows (cf. [Duffield *et al.*, 1992, Prop. 6.1] or [Duffield and Werner, 1992a, Prop. 3.1] that  $\langle \varphi_t^h(\omega), B \rangle = \langle \omega, U_t^h B (U_t^h)^* \rangle$  for some unitary  $U_t^h \in \mathcal{B}$ . For example, if  $h = \hat{A}$  then  $U_t^h = \exp(itA)$ .

<sup>298</sup>More generally, a Poisson space. The structure of  $\mathcal{P}(\mathcal{B})$  as a Poisson space was introduced by Landsman [1997; 1998] without recourse to the full state space or the work of Duffield and Werner [1992a].

<sup>299</sup>Equipped with a multiple of the so-called Fubini–Study symplectic structure; see [Landsman, 1998] or any decent book on differential geometry for this notion. This claim is immediate from footnote 260. More generally, the pure state space of  $M_n(\mathbb{C})$  is the projective space  $\mathbb{P}\mathbb{C}^n$ , which again becomes equipped with the Fubini–Study symplectic structure. This is even true for  $n = \infty$  if one defines  $M_\infty(\mathbb{C})$  as the  $C^*$ -algebra of compact operators on a separable Hilbert space  $\mathcal{H}$ : in that case one has  $\mathcal{P}(M_\infty(\mathbb{C})) \cong \mathbb{P}\mathcal{H}$ . Cf. [Cantoni, 1977; Cirelli *et al.*, 1983; Cirelli *et al.*, 1990; Landsman, 1998; Ashtekar and Schilling, 1999; Marmo *et al.*, 2005], etc.

symplectic leaves of  $M$  can be almost anything, the coincidence in question does not hold.

However, there exists a compatibility condition between the transition probability structure and the Poisson structure, which is shared by classical and quantum theory. This is the property of *unitarity* of a Hamiltonian flow, which in the present setting we formulate as follows.<sup>300</sup> First, in quantum theory with algebra of observables  $\mathcal{B}$  we define time-evolution (in the sense of an automorphic action of the abelian group  $\mathbb{R}$  on  $\mathcal{B}$ , i.e. a one-parameter group  $\alpha$  of automorphisms on  $\mathcal{B}$ ) to be *Hamiltonian* when  $A(t) = \alpha_t(A)$  satisfies the Heisenberg equation  $i\hbar dA/dt = [A, H]$  for some self-adjoint element  $H \in \mathcal{B}$ . The corresponding flow on  $\mathcal{P}(\mathcal{B})$  — i.e.  $\omega_t(A) = \omega(A(t))$  — is equally well said to be Hamiltonian in that case. In classical mechanics with Poisson manifold  $M$  we similarly say that a flow on  $M$  is Hamiltonian when it is the flow of a Hamiltonian vector field  $\xi_h$  for some  $h \in C^\infty(M)$ . (Equivalently, the time-evolution of the observables  $f \in C^\infty(M)$  is given by  $df/dt = \{h, f\}$ ; cf. (18) etc.) The point is that in either case the flow is unitary in the sense that

$$(41) \quad p(\rho(t), \sigma(t)) = p(\rho, \sigma)$$

for all  $t$  and all  $\rho, \sigma \in P$  with  $P = \mathcal{P}(\mathcal{B})$  (equipped with the transition probabilities (27) and the Poisson bracket (38)) or  $P = M$  (equipped with the transition probabilities (31) and any Poisson bracket).<sup>301</sup>

In both cases  $P = \mathcal{P}(\mathcal{B})$  and  $P = M$ , a Hamiltonian flow has the property (which is immediate from the definition of a symplectic leaf) that for all (finite) times  $t$  a point  $\omega(t)$  lies in the same symplectic leaf of  $P$  as  $\omega = \omega(0)$ . In particular, in quantum theory  $\omega(t)$  and  $\omega$  must lie in the same sector. In the quantum theory of infinite systems an automorphic time-evolution is rarely Hamiltonian, but one reaches a similar conclusion under a weaker assumption. Namely, if a given one-parameter group of automorphisms  $\alpha$  on  $\mathcal{B}$  is *implemented* in the GNS-representation  $\pi_\omega(\mathcal{B})$  for some  $\omega \in \mathcal{P}(\mathcal{B})$ ,<sup>302</sup> then  $\omega(t)$  and  $\omega$  lie in the same sector and hence in the same symplectic leaf of  $\mathcal{P}(\mathcal{B})$ .

To illustrate these concepts, let us return to our continuous field of  $C^*$ -algebras  $\mathcal{A}^{(c)}$ ; cf. (2). It may not come as a great surprise that the canonical  $C^*$ -algebraic transition probabilities (27) on the pure state space of each fiber algebra  $\mathcal{A}_{1/N}^{(c)}$  for  $N < \infty$  converge to the classical transition probabilities (31) on the commutative limit algebra  $\mathcal{A}_0^{(c)}$ . Similarly, the  $C^*$ -algebraic Poisson structure (38) on each  $\mathcal{P}(\mathcal{A}_{1/N}^{(c)})$  converges to zero. However, we know from the limit  $\hbar \rightarrow 0$  of quantum mechanics that in generating classical behaviour on the limit algebra of a continuous field of  $C^*$ -algebras one should rescale the commutators; see Subsection 4.3

<sup>300</sup>All this can be boosted into an axiomatic structure into which both classical and quantum theory fit; see [Landsman, 1997; 1998].

<sup>301</sup>In quantum theory the flow is defined for any  $t$ . In classical dynamics, (41) holds for all  $t$  for which  $\rho(t)$  and  $\sigma(t)$  are defined, cf. footnote 253.

<sup>302</sup>This assumption means that there exists a unitary representation  $t \mapsto U_t$  of  $\mathbb{R}$  on  $\mathcal{H}_\omega$  such that  $\pi_\omega(\alpha_t(A)) = U_t \pi_\omega(A) U_t^*$  for all  $A \in \mathcal{B}$  and all  $t \in \mathbb{R}$ .

and Section 5. Thus we replace the Poisson bracket (38) for  $\mathcal{A}_{1/N}^{(c)}$  by

$$(42) \quad \{f, g\}(\omega) = iN\omega([df_\omega, dg_\omega]).$$

Thus rescaled, the Poisson brackets on the spaces  $\mathcal{P}(\mathcal{A}_{1/N}^{(c)})$  turn out to converge to the canonical Poisson bracket (38) on  $\mathcal{P}(\mathcal{A}_0^{(c)}) = \mathcal{S}(\mathcal{A}_1)$ , instead of the zero bracket expected from the commutative nature of the limit algebra  $\mathcal{A}_0^{(c)}$ . Consequently, the symplectic leaves of the *full* state space  $\mathcal{S}(\mathcal{A}_1)$  of the fiber algebra  $\mathcal{A}_1^{(c)}$  become the symplectic leaves of the *pure* state space  $\mathcal{S}(\mathcal{A}_1)$  of the fiber algebra  $\mathcal{A}_0^{(c)}$ . This is undoubtedly indicative of the origin of classical phase spaces and their Poisson structures in quantum theory.

More precisely, we have the following result [Duffield and Werner, 1992a]:

*If  $A = (A_0, A_1, A_2, \dots)$  and  $A' = (A'_0, A'_1, A'_2, \dots)$  are continuous sections of  $\mathcal{A}^{(c)}$  defined by symmetric sequences,<sup>303</sup> then the sequence*

$$(43) \quad (\{A_0, A'_0\}, i[A_1, A'_1], \dots, iN[A_N, A'_N], \dots)$$

*defines a continuous section of  $\mathcal{A}^{(c)}$ .*

This follows from an easy computation. In other words, although the sequence of commutators  $[A_N, A'_N]$  converges to zero, the rescaled commutators  $iN[A_N, A'_N] \in \mathcal{A}_N$  converge to the macroscopic observable  $\{A_0, A'_0\} \in \mathcal{A}_0^{(c)} = C(\mathcal{S}(\mathcal{A}_1))$ . Although it might seem perverse to reinterpret this result on the classical limit of a large quantum system in terms of quantization (which is the *opposite* of taking the classical limit), it is formally possible to do so (cf. Section 4.3) if we put

$$(44) \quad \hbar = \frac{1}{N}.$$

Using the axiom of choice if necessary, we devise a procedure that assigns a continuous section  $A = (A_0, A_1, A_2, \dots)$  of our field to a given function  $A_0 \in \mathcal{A}_0^{(c)}$ . We write this as  $A_N = \mathcal{Q}_{\frac{1}{N}}(A_0)$ , and similarly  $A'_N = \mathcal{Q}_{\frac{1}{N}}(A'_0)$ . This choice need not be such that the sequence (43) is assigned to  $\{A_0, A'_0\}$ , but since the latter is the unique limit of (43), it must be that

$$(45) \quad \lim_{N \rightarrow \infty} \left\| iN \left[ \mathcal{Q}_{\frac{1}{N}}(A_0), \mathcal{Q}_{\frac{1}{N}}(A'_0) \right] - \mathcal{Q}_{\frac{1}{N}}(\{A_0, A'_0\}) \right\| = 0.$$

Also note that (27) is just (12). Consequently (cf. (25) and surrounding text):

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<sup>303</sup>The result does not hold for all continuous sections (i.e. for all approximately symmetric sequences), since, for example, the limiting functions  $A_0$  and  $A'_0$  may not be differentiable, so that their Poisson bracket does not exist. This problem occurs in all examples of deformation quantization. However, the class of sequences for which the claim is valid is larger than the symmetric ones alone. A sufficient condition on  $A$  and  $B$  for (43) to make sense is that  $A_N = \sum_{M \leq N} j_{NM}(A_M^{(N)})$  (with  $A_M^{(N)} \in \mathcal{A}_1^M$ ), such that  $\lim_{N \rightarrow \infty} A_M^{(N)}$  exists (in norm) and  $\sum_{M=1}^{\infty} M \sup_{N \geq M} \{\|A_M^{(N)}\|\} < \infty$ . See [Duffield and Werner, 1992a].

The continuous field of  $C^*$ -algebras  $\mathcal{A}^{(c)}$  defined by (2) and approximately symmetric sequences (and their limits) as continuous sections yields a deformation quantization of the phase space  $\mathcal{S}(\mathcal{A}_1)$  (equipped with the Poisson bracket (38)) for any quantization map  $\mathcal{Q}$ .

For the dynamics this implies:

Let  $H = (H_0, H_1, H_2, \dots)$  be a continuous section of  $\mathcal{A}^{(c)}$  defined by a symmetric sequence,<sup>304</sup> and let  $A = (A_0, A_1, A_2, \dots)$  be an arbitrary continuous section of  $\mathcal{A}^{(c)}$  (i.e. an approximately symmetric sequence). Then the sequence

$$(46) \quad (A_0(t), e^{iH_1 t} A_1 e^{-iH_1 t}, \dots, e^{iNH_N t} A_N e^{-iNH_N t}, \dots),$$

where  $A_0(t)$  is the solution of the equations of motion with classical Hamiltonian  $H_0$ ,<sup>305</sup> defines a continuous section of  $\mathcal{A}^{(c)}$ .

In other words, for bounded symmetric sequences of Hamiltonians  $H_N$  the quantum dynamics restricted to macroscopic observables converges to the classical dynamics with Hamiltonian  $H_0$ . Compare the positions of  $\hbar$  and  $N$  in (12) and (46), respectively, and rejoice in the reconfirmation of (44).

In contrast, the quasilocal observables are *not* well behaved as far as the  $N \rightarrow \infty$  limit of the dynamics defined by such Hamiltonians is concerned. Namely, if  $(A_0, A_1, \dots)$  is a section of the continuous field  $\mathcal{A}^{(q)}$ , and  $(H_1, H_2, \dots)$  is any bounded symmetric sequence of Hamiltonians, then the sequence

$$(e^{iH_1 t} A_1 e^{-iH_1 t}, \dots, e^{iNH_N t} A_N e^{-iNH_N t}, \dots)$$

has no limit for  $N \rightarrow \infty$ , in that it cannot be extended by some  $A_0(t)$  to a continuous section of  $\mathcal{A}^{(q)}$ . Indeed, this was the very reason why macroscopic observables were originally introduced in this context [Rieckers, 1984; Morchio and Strocchi, 1987; Bona, 1988; Unnerstall, 1990a; Raggio and Werner, 1989; Duffield and Werner, 1992a]. Instead, the natural finite- $N$  Hamiltonians for which the limit  $N \rightarrow \infty$  of the time-evolution on  $\mathcal{A}_1^N$  exists as a one-parameter automorphism group on  $\mathcal{A}^{(q)}$  satisfy an appropriate locality condition, which excludes the global averages defining symmetric sequences.

## 6.6 Epilogue: Macroscopic observables and the measurement problem

In a renowned paper, Hepp [1972] suggested that macroscopic observables and superselection rules should play a role in the solution of the measurement problem of

<sup>304</sup>Once again, the result in fact holds for a larger class of Hamiltonians, namely the ones satisfying the conditions specified in footnote 303 [Duffield and Werner, 1992a]. The assumption that each Hamiltonian  $H_N$  lies in  $\mathcal{A}_1^N$  and hence is bounded is natural in lattice models, but is undesirable in general.

<sup>305</sup>See (18) and surrounding text.



quantum mechanics. He assumed that a macroscopic apparatus may be idealized as an infinite quantum system, whose algebra of observables  $\mathcal{A}_A$  has disjoint pure states. Referring to our discussion in Subsection 2.5 for context and notation, Hepp's basic idea (for which he claimed no originality) was that as a consequence of the measurement process the initial state vector  $\Omega_I = \sum_n c_n \Psi_n \otimes I$  of system plus apparatus evolves into a final state vector  $\Omega_F = \sum_n c_n \Psi_n \otimes \Phi_n$ , in which each  $\Phi_n$  lies in a different superselection sector of the Hilbert space of the apparatus (in other words, the corresponding states  $\varphi_n$  on  $\mathcal{A}_A$  are mutually disjoint). Consequently, although the initial state  $\omega_I$  is pure, the final state  $\omega_F$  is mixed. Moreover, because of the disjointness of the  $\omega_n$  the final state  $\omega_F$  has a unique decomposition  $\omega_F = \sum_n |c_n|^2 \psi_n \otimes \varphi_n$  into pure states, and therefore admits a bona fide ignorance interpretation. Hepp therefore claimed with some justification that the measurement "reduces the wave packet", as desired in quantum measurement theory.

Even apart from the usual conceptual problem of passing from the collective of all terms in the final mixture to one actual measurement outcome, Hepp himself indicated a serious mathematical problem with this program. Namely, if the initial state is pure it must lie in a certain superselection sector (or equivalence class of states); but then the final state must lie in the very same sector if the time-evolution is Hamiltonian, or, more generally, automorphic (as we have seen in the preceding subsection). Alternatively, it follows from a more general lemma Hepp [1972] himself proved:

*If two states  $\rho, \sigma$  on a  $C^*$ -algebra  $\mathcal{B}$  are disjoint and  $\alpha : \mathcal{B} \rightarrow \mathcal{B}$  is an automorphism of  $\mathcal{B}$ , then  $\rho \circ \alpha$  and  $\sigma \circ \alpha$  are disjoint, too.*

To reach the negative conclusion above, one takes  $\mathcal{B}$  to be the algebra of observables of system and apparatus jointly, and computes back in time by choosing  $\alpha = \alpha_{t_F - t_I}^{-1}$ , where  $\alpha_t$  is the one-parameter automorphism group on  $\mathcal{B}$  describing the joint time-evolution of system and apparatus (and  $t_I$  and  $t_F$  are the initial and final times of the measurement, respectively). However, Hepp pointed out that this conclusion may be circumvented if one admits the possibility that a measurement takes infinitely long to complete. For the limit  $A \mapsto \lim_{t \rightarrow \infty} \alpha_t(A)$  (provided it exists in a suitable sense, e.g., weakly) does not necessarily yield an automorphism of  $\mathcal{B}$ . Hence a state — evolving in the Schrödinger picture by  $\omega_t(A) \equiv \omega(\alpha_t(A))$  — may leave its sector in infinite time, a possibility Hepp actually demonstrated in a range of models; see also [Frigerio, 1974; Whitten-Wolfe and Emch, 1976; Araki, 1980; Bona, 1980; Hannabuss, 1984; Bub, 1988; Landsman, 1991; Frasca, 2003; 2004], and many other papers.

Despite the criticism that has been raised against the conclusion that a quantum-mechanical measurement requires an infinite apparatus and must take infinite time [Bell, 1975; Robinson, 1994; Landsman, 1995], and despite the fact that this procedure is quite against the spirit of von Neumann [1932], in whose widely accepted description measurements are practically instantaneous, this conclusion resonates well with the modern idea that quantum theory is universally valid and the classical

world has no absolute existence; cf. the Introduction. Furthermore, a quantum-mechanical measurement is nothing but a specific interaction, comparable with a scattering process; and it is quite uncontroversial that such a process takes infinite time to complete. Indeed, what would it mean for scattering to be over after some finite time? Which time? As we shall see in the next section, the theory of decoherence requires the limit  $t \rightarrow \infty$  as well, and largely for the same mathematical reasons. There as well as in Hepp's approach, the limiting behaviour actually tends to be approached very quickly (on the pertinent time scale), and one needs to let  $t \rightarrow \infty$  merely to make terms  $\sim \exp -\gamma t$  (with  $\gamma > 0$ ) zero rather than just very small. See also [Primas, 1997] for a less pragmatic point of view on the significance of this limit.

A more serious problem with Hepp's approach lies in his assumption that the time-evolution on the quasilocal algebra of observables of the infinite measurement apparatus (which in our class of examples would be  $\mathcal{A}_0^{(q)}$ ) is automorphic. This, however, is by no means always the case; cf. the references listed near the end of Subsection 6.5. As we have seen, for certain natural Hamiltonian (and hence automorphic) time-evolutions at finite  $N$  the dynamics *has no limit*  $N \rightarrow \infty$  on the algebra of quasilocal observables — let alone an automorphic one.

Nonetheless, Hepp's conclusion remains valid if we use the algebra  $\mathcal{A}_0^{(c)}$  of macroscopic observables, on which (under suitable assumptions — see Subsection 6.5) Hamiltonian time-evolution on  $\mathcal{A}_1^N$  *does* have a limit as  $N \rightarrow \infty$ . For, as pointed out in Subsection 6.3, each superselection sector of  $\mathcal{A}_0^{(q)}$  defines and is defined by a pure state on  $\mathcal{A}_1$ , which in turn defines a sector of  $\mathcal{A}_0^{(c)}$ . Now the latter sector is simply a point in the pure state space  $\mathcal{S}(\mathcal{A}_1)$  of the commutative  $C^*$ -algebra  $\mathcal{A}_0^{(c)}$ , so that Hepp's lemma quoted above boils down to the claim that if  $\rho \neq \sigma$ , then  $\rho \circ \alpha \neq \sigma \circ \alpha$  for any automorphism  $\alpha$ . This, of course, is a trivial property of any Hamiltonian time-evolution, and it follows once again that a transition from a pure pre-measurement state to a mixed post-measurement state on  $\mathcal{A}_0^{(c)}$  is impossible in finite time. To avoid this conclusion, one should simply avoid the limit  $N \rightarrow \infty$ , which is the root of the  $t \rightarrow \infty$  limit; see [Janssens, 2005].

What, then, does all this formalism mean for Schrödinger's cat? In our opinion, it confirms the impression that the appearance of a paradox rests upon an equivocation. Indeed, the problem arises because one oscillates between two mutually exclusive interpretations.<sup>306</sup>

*Either* one is a bohemian theorist who, in vacant or in pensive mood, puts off his or her glasses and merely contemplates whether the cat is dead or alive. Such a person studies the cat exclusively from the point of view of its macroscopic observables, so that he or she has to use a post-measurement state  $\omega_F^{(c)}$  on the algebra  $\mathcal{A}_0^{(c)}$ . If  $\omega_F^{(c)}$  is pure, it lies in  $\mathcal{P}(\mathcal{A}_1)$  (unless the pre-measurement state was mixed). Such a state corresponds to a single superselection sector  $[\omega_F^{(q)}]$  of  $\mathcal{A}_0^{(q)}$ , so that the cat is dead or alive. If, on the other hand,  $\omega_F^{(c)}$  is mixed (which

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<sup>306</sup>Does *complementarity* re-enter through the back door?

is what occurs if Schrödinger has his way), there is no problem in the first place: at the level of macroscopic observables one merely has a statistical description of the cat.

Or one is a hard-working experimental physicist of formidable power, who investigates the detailed microscopic constitution of the cat. For him or her the cat is always in a pure state on  $\mathcal{A}_1^N$  for some large  $N$ . This time the issue of life and death is not a matter of lazy observation and conclusion, but one of sheer endless experimentation and computation. From the point of view of such an observer, nothing is wrong with the cat being in a coherent superposition of two states that are actually quite close to each other microscopically — at least for the time being.

Either way, *the riddle does not exist* (Wittgenstein, TLP, §6.5).

## 7 WHY CLASSICAL STATES AND OBSERVABLES?

‘We have found a strange footprint on the shores of the unknown. We have devised profound theories, one after another, to account for its origins. At last, we have succeeded in reconstructing the creature that made the footprint. And lo! It is our own.’ [Eddington, 1920, 200–201]

The conclusion of Sections 5 and 6 is that quantum theory may give rise to classical behaviour *in certain states* and *with respect to certain observables*. For example, we have seen that in the limit  $\hbar \rightarrow 0$  coherent states and operators of the form  $\mathcal{Q}_\hbar(f)$ , respectively, are appropriate, whereas in the limit  $N \rightarrow \infty$  one should use classical states (*nomen est omen!*) as defined in Subsection 6.2 and macroscopic observables. If, instead, one uses superpositions of such states, or observables with the wrong limiting behaviour, no classical physics emerges. Thus the question remains why the world at large should happen to be in such states, and why we turn out to study this world with respect to the observables in question. This question found its original incarnation in the measurement problem (cf. Subsection 2.5), but this problem is really a figure-head for a much wider difficulty.

Over the last 25 years,<sup>307</sup> two profound and original answers to this question have been proposed.

### 7.1 Decoherence

The first goes under the name of *decoherence*. Pioneering papers include [van Kampen, 1954; Zeh, 1970; Zurek, 1981; 1982],<sup>308</sup> and [Joos and Zeh, 1985], and some recent reviews are [Bub, 1999; Auletta, 2001; Joos *et al.*, 2003; Zurek, 2003; Blanchard and Olkiewicz, 2003; Bacciagaluppi, 2004] and [Schlosshauer, 2004].<sup>309</sup>

<sup>307</sup>Though some say the basic idea of decoherence goes back to Heisenberg and Ludwig.

<sup>308</sup>See also [Zurek, 1991] and the subsequent debate in *Physics Today* [Zurek, 1993], which drew wide attention to decoherence.

<sup>309</sup>The website [http://almaak.usc.edu/~tbrun/Data/decoherence\\_list.html](http://almaak.usc.edu/~tbrun/Data/decoherence_list.html) contains an extensive list of references on decoherence.

More references will be given in due course. The existence (and excellence) of these reviews obviates the need for a detailed treatment of decoherence in this article, all the more so since at the time of writing this approach appears to be in a transitional stage, conceptually as well as mathematically (as will be evident from what follows). Thus we depart from the layout of our earlier chapters and restrict ourselves to a few personal comments.

1. Mathematically, decoherence boils down to the idea of adding one more link to the von Neumann chain (see Subsection 2.5) beyond  $S + A$  (i.e. the system and the apparatus). Conceptually, however, there is a major difference between decoherence and older approaches that took such a step: whereas previously (e.g., in the hands of von Neumann, London and Bauer, Wigner, etc.)<sup>310</sup> the chain *converged towards the observer*, in decoherence it *diverges away from the observer*. Namely, the third and final link is now taken to be the *environment* (taken in a fairly literal sense in agreement with the intuitive meaning of the word). In particular, in realistic models the environment is treated as an infinite system (necessitating the limit  $N \rightarrow \infty$ ), which has the consequence that (in simple models where the pointer has discrete spectrum) the post-measurement state  $\sum_n c_n \Psi_n \otimes \Phi_n \otimes \chi_n$  (in which the  $\chi_n$  are mutually orthogonal) is only reached in the limit  $t \rightarrow \infty$ . However, as already mentioned in Subsection 6.6, infinite time is only needed mathematically in order to make terms of the type  $\sim \exp -\gamma t$  (with  $\gamma > 0$ ) zero rather than just very small: in many models the inner products  $(\chi_n, \chi_m)$  are actually negligible for  $n \neq m$  within surprisingly short time scales.<sup>311</sup>

If only in view of the need for limits of the type  $N \rightarrow \infty$  (for the environment) and  $t \rightarrow \infty$ , in our opinion decoherence is best linked to stance 1 of the Introduction: its goal is to explain the approximate appearance of the classical world from quantum mechanics seen as a universally valid theory. However, decoherence has been claimed to support almost any opinion on the foundations of quantum mechanics; cf. [Bacciagaluppi, 2004] and [Schlosshauer, 2004] for a critical overview and also see Point 3 below.

2. Originally, decoherence entered the scene as a proposed solution to the measurement problem (in the precise form stated at the end of Subsection 2.5). For the restriction of the state  $\sum_n c_n \Psi_n \otimes \Phi_n \otimes \chi_n$  to  $S + A$  (i.e. its trace over the degrees of freedom of the environment) is mixed in the limit  $t \rightarrow \infty$ , which means that the quantum-mechanical interference between the states  $\Psi_n \otimes \Phi_n$  for different values of  $n$  has become ‘delocalized’ to the environment, and accordingly is irrelevant if the latter is not observed (i.e. omitted from the description). Unfortunately, the application of the ignorance interpretation of the mixed post-measurement state of  $S + A$  is illegal even from the point of view of stance 1 of the Introduction. The ignorance interpretation

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<sup>310</sup>See [Wheeler and Zurek, 1983].

<sup>311</sup>Cf. Tables 3.1 and 3.2 on pp. 66–67 of [Joos *et al.*, 2003].

is only valid if the environment is kept within the description *and* is classical (in having a commutative  $C^*$ -algebra of observables). The latter assumption [Primas, 1983], however, makes the decoherence solution to the measurement problem circular.<sup>312</sup>

In fact, as quite rightly pointed out by Bacciagaluppi [2004], decoherence actually *aggravates* the measurement problem. Where previously this problem was believed to be man-made and relevant only to rather unusual laboratory situations (important as these might be for the foundations of physics), it has now become clear that “measurement” of a quantum system *by the environment* (instead of by an experimental physicist) happens everywhere and all the time: hence it remains even more miraculous than before that there is a single outcome after each such measurement. Thus decoherence as such does not provide a solution to the measurement problem [Leggett, 2002];<sup>313</sup> Adler, 2003; Joos and Zeh, 2003], but is in actual fact parasitic on such a solution.

3. There have been various responses to this insight. The dominant one has been to combine decoherence with some interpretation of quantum mechanics: decoherence then finds a home, while conversely the interpretation in question is usually enhanced by decoherence. In this context, the most popular of these has been the many-worlds interpretation, which, after decades of obscurity and derision, suddenly started to be greeted with a flourish of trumpets in the wake of the popularity of decoherence. See, for example, [Saunders, 1993; 1995; Joos *et al.*, 2003] and [Zurek, 2003]. In quantum cosmology circles, the consistent histories approach has been a popular partner to decoherence, often in combination with many worlds; see below. The importance of decoherence in the modal interpretation has been emphasized by Dieks [1989b] and Bene and Dieks [2002], and practically all authors on decoherence find the opportunity to pay some lip-service to Bohr in one way or another. See [Bacciagaluppi, 2004] and [Schlosshauer, 2004] for a critical assessment of all these combinations.

In our opinion, none of the established interpretations of quantum mechanics will do the job, leaving room for genuinely new ideas. One such idea is the *return of the environment*: instead of “tracing it out”, as in the original setting of decoherence theory, the environment should *not* be ignored! The

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<sup>312</sup>On the other hand, treating the environment *as if* it were classical might be an improvement on the Copenhagen ideology of treating the measurement apparatus *as if* it were classical (cf. Section 3).

<sup>313</sup>In fact, Leggett’s argument only applies to strawman 3 of the Introduction and loses its force against stance 1. For his argument is that decoherence just removes the *evidence* for a given state (of Schrödinger’s cat type) to be a superposition, and accuses those claiming that this solves the measurement problem of committing the logical fallacy that removal of the evidence for a crime would undo the crime. But according to stance 1 *the crime is only defined relative to the evidence!* Leggett is quite right, however, in insisting on the ‘from “and” to “or” problem’ mentioned at the end of the Introduction.

essence of measurement has now been recognized to be the *redundancy* of the outcome (or “record”) of the measurement in the environment. It is this very redundancy of information about the underlying quantum object that “objectifies” it, in that the information becomes accessible to a large number of observers without necessarily disturbing the object<sup>314</sup> [Zurek, 2003; Olivier *et al.* 2004; Blume-Kohout and Zurek, 2004; 2005]. This insight (called “Quantum Darwinism”) has given rise to the “existential” interpretation of quantum mechanics due to Zurek [2003].

4. Another response to the failure of decoherence (and indeed all other approaches) to solve the measurement problem (in the sense of failing to win a general consensus) has been of a somewhat more pessimistic (or, some would say, pragmatic) kind: all attempts to explain the quantum world are given up, yielding to the point of view that ‘the appropriate aim of physics at the fundamental level then becomes the representation and manipulation of information’ [Bub, 2004]. Here ‘measuring instruments ultimately remain black boxes at some level’, and one concludes that all efforts to *understand* measurement (or, for that matter, EPR-correlations) are futile and pointless.<sup>315</sup>
  
5. Night thoughts of a quantum physicist, then?<sup>316</sup> Not quite. Turning vice into virtue: rather than solving the measurement problem, the true significance of the decoherence program is that it gives conditions under which there is no measurement problem! Namely, foregoing an explanation of the transition from the state  $\sum_n c_n \Psi_n \otimes \Phi_n \otimes \chi_n$  of  $S + A + \mathcal{E}$  to a single one of the states  $\Psi_n \otimes \Phi_n$  of  $S + A$ , at the heart of decoherence is the claim that each of the latter states is *robust* against coupling to the environment (provided the Hamiltonian is such that  $\Psi_n \otimes \Phi_n$  tensored with some initial state  $\mathcal{I}_{\mathcal{E}}$  of the environment indeed evolves into  $\Psi_n \otimes \Phi_n \otimes \chi_n$ , as assumed so far). This implies that each state  $\Psi_n \otimes \Phi_n$  remains pure after coupling to the environment and subsequent restriction to the original system plus apparatus, so that at the end of the day the environment has had no influence on it. In other words, the real point of decoherence is the phenomenon of *einselection* (for *environment-induced superselection*), where a state is ‘einselected’ precisely when (given some interaction Hamiltonian) it possesses the stability property just mentioned. The claim, then, is that einselected states are often classical, or at least that classical states (in the sense mentioned at the beginning of this section) are classical precisely because they are robust against coupling to the environment. Provided this scenario indeed gives

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<sup>314</sup>Such objectification is claimed to yield an ‘operational definition of existence’ [Zurek, 2003, 749].

<sup>315</sup>It is indeed in describing the transformation of quantum information (or entropy) to classical information during measurement that decoherence comes to its own and exhibits some of its greatest strength. Perhaps for this reason such thinking pervades also Zurek [2003].

<sup>316</sup>[Kent, 2000]. Pun on the title of McCormmach [1982].

rise to the classical world (which remains to be shown in detail), it gives a dynamical explanation of it. But even short of having achieved this goal, the importance of the notion of einselection cannot be overstated; in our opinion, it is the most important and powerful idea in quantum theory since entanglement (which einselection, of course, attempts to undo!).

6. The measurement problem, and the associated distinction between system and apparatus on the one hand and environment on the other, can now be *omitted* from decoherence theory. Continuing the discussion in Subsection 3.4, the goal of decoherence should simply be to find the robust or einselected states of a object  $\mathcal{O}$  coupled to an environment  $\mathcal{E}$ , as well as the induced dynamics thereof (given the time-evolution of  $\mathcal{O} + \mathcal{E}$ ). This search, however, must include the correct *identification* of the object  $\mathcal{O}$  within the total  $\mathcal{S} + \mathcal{E}$ , namely as a subsystem that actually *has* such robust states. Thus the Copenhagen idea that the Heisenberg cut between object and apparatus be movable (cf. Subsection 3.2) will not, in general, extend to the “Primas–Zurek” cut between object and environment. In traditional physics terminology, the problem is to find the right “dressing” of a quantum system so as to make at least some of its states robust against coupling to its environment [Amann and Primas, 1997; Brun and Hartle, 1999; Omnès, 2002]. In other words: *What is a system?* To mark this change in perspective, we now change notation from  $\mathcal{O}$  (for “object”) to  $\mathcal{S}$  (for “system”). Various tools for the solution of this problem within the decoherence program have now been developed — with increasing refinement and also increasing reliance on concepts from information theory [Zurek, 2003] — but the right setting for it seems the formalism of consistent histories, see below.
7. Various dynamical regimes haven been unearthed, each of which leads to a different class of robust states [Joos *et al.*, 2003; Zurek, 2003; Schlosshauer, 2004]. Here  $H_{\mathcal{S}}$  is the system Hamiltonian,  $H_I$  is the interaction Hamiltonian between system and environment, and  $H_{\mathcal{E}}$  is the environment Hamiltonian. As stated, no reference to measurement, object or apparatus need be made here.
  - In the regime  $H_{\mathcal{S}} \ll H_I$ , for suitable Hamiltonians the robust states are the traditional pointer states of quantum measurement theory. This regime conforms to von Neumann’s [1932] idea that quantum measurements be almost instantaneous. If, moreover,  $H_{\mathcal{E}} \ll H_I$  as well — with or without a measurement context — then the decoherence mechanism turns out to be universal in being independent of the details of  $\mathcal{E}$  and  $H_{\mathcal{E}}$  [Strunz *et al.*, 2003].
  - If  $H_{\mathcal{S}} \approx H_I$ , then (at least in models of quantum Brownian motion) the robust states are coherent states (either of the traditional Schrödinger type, or of a more general nature as defined in Subsection 5.1); see [Zurek *et al.*, 1993] and [Zurek, 2003]. This case is, of course, of supreme

importance for the physical relevance of the results quoted in our Section 5 above, and — if only for this reason — decoherence theory would benefit from more interaction with mathematically rigorous results on quantum stochastic analysis.<sup>317</sup>

- Finally, if  $H_S \gg H_I$ , then the robust states turn out to be eigenstates of the system Hamiltonian  $H_S$  [Paz and Zurek, 1999; Ollivier *et al.*, 2004]. In view of our discussion of such states in Subsections 5.5 and 5.6, this shows that robust states are not necessarily classical. It should be mentioned that in this context decoherence theory largely coincides with standard atomic physics, in which the atom is taken to be the system  $\mathcal{S}$  and the radiation field plays the role of the environment  $\mathcal{E}$ ; see [Gustafson and Sigal, 2003] for a mathematically minded introductory treatment and [Bach *et al.*, 1998; 1999] for a full (mathematical) meal.
8. Further to the above clarification of the role of energy eigenstates, decoherence also has had important things to say about quantum chaos [Zurek, 2003; Joos *et al.*, 2003]. Referring to our discussion of wave packet revival in Subsection 2.4, we have seen that in atomic physics wave packets do not behave classically on long time scales. Perhaps surprisingly, this is even true for certain chaotic macroscopic systems: cf. the case of Hyperion mentioned in the Introduction and at the end of Subsection 5.2. Decoherence now replaces the underlying superposition by a classical probability distribution, which reflects the chaotic nature of the limiting classical dynamics. Once again, the transition from the pertinent pure state of system plus environment to *a single* observed system state remains clouded in mystery. But granted this transition, decoherence sheds new light on classical chaos and circumvents at least the most flagrant clashes with observation.<sup>318</sup>
  9. Robustness and einselection form the state side or Schrödinger picture of decoherence. Of course, there should also be a corresponding observable side or Heisenberg picture of decoherence. But the transition between the two pictures is more subtle than in the quantum mechanics of closed systems. In the Schrödinger picture, the whole point of einselection is that most pure states simply disappear from the scene. This may be beautifully visualized on the example of a two-level system with Hilbert space  $\mathcal{H}_S = \mathbb{C}^2$  [Zurek, 2003]. If  $\uparrow$  and  $\downarrow$  (cf. (33)) happen to be the robust vector states of the system after coupling to an appropriate environment, and if we identify the corresponding density matrices with the north-pole  $(0, 0, 1) \in B^3$  and the south-pole  $(0, 0, -1) \in B^3$ , respectively (cf. (3)), then following decoherence all other states move towards the axis connecting the north- and south poles

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<sup>317</sup>Cf. [Davies, 1976; Accardi *et al.*, 1990; Parthasarathy, 1992; Streater, 2000; Kümmerer, 2002; Maassen, 2003], etc.

<sup>318</sup>It should be mentioned, though, that any successful mechanism explaining the transition from quantum to classical should have this feature, so that at the end of the day decoherence might turn out to be a red herring here.



(i.e. the intersection of the  $z$ -axis with  $B^3$ ) as  $t \rightarrow \infty$ . In the Heisenberg picture, this disappearance of all pure states except two corresponds to the reduction of the full algebra of observables  $M_2(\mathbb{C})$  of the system to its diagonal (and hence commutative) subalgebra  $\mathbb{C} \oplus \mathbb{C}$  in the same limit. For it is only the latter algebra that contains enough elements to distinguish  $\uparrow$  and  $\downarrow$  without containing observables detecting interference terms between these pure states.

10. To understand this in a more abstract and general way, we recall the mathematical relationship between pure states and observables [Landsman, 1998]. The passage from a  $C^*$ -algebra  $\mathcal{A}$  of observables of a given system to its pure states is well known: as a set, the pure state space  $\mathcal{P}(\mathcal{A})$  is the extreme boundary of the total state space  $\mathcal{S}(\mathcal{A})$  (cf. footnote 259). In order to reconstruct  $\mathcal{A}$  from  $\mathcal{P}(\mathcal{A})$ , the latter needs to be equipped with the structure of a transition probability space (see Subsection 6.3) through (27). Each element  $A \in \mathcal{A}$  defines a function  $\hat{A}$  on  $\mathcal{P}(\mathcal{A})$  by  $\hat{A}(\omega) = \omega(A)$ . Now, in the simple case that  $\mathcal{A}$  is finite-dimensional (and hence a direct sum of matrix algebras), one can show that each function  $\hat{A}$  is a finite linear combination of the form  $\hat{A} = \sum_i p_{\omega_i}$ , where  $\omega_i \in \mathcal{P}(\mathcal{A})$  and the elementary functions  $p_\rho$  on  $\mathcal{P}(\mathcal{A})$  are defined by  $p_\rho(\sigma) = p(\rho, \sigma)$ . Conversely, each such linear combination defines a function  $\hat{A}$  for some  $A \in \mathcal{A}$ . Thus the elements of  $\mathcal{A}$  (seen as functions on the pure state space  $\mathcal{P}(\mathcal{A})$ ) are just the transition probabilities and linear combinations thereof. The algebraic structure of  $\mathcal{A}$  may then be reconstructed from the structure of  $\mathcal{P}(\mathcal{A})$  as a Poisson space with a transition probability (cf. Subsection 6.5). In this sense  $\mathcal{P}(\mathcal{A})$  uniquely determines the algebra of observables of which it is the pure state space. For example, the space consisting of two points with classical transition probabilities (31) leads to the commutative algebra  $\mathcal{A} = \mathbb{C} \oplus \mathbb{C}$ , whereas the unit two-sphere in  $\mathbb{R}^3$  with transition probabilities (32) yields  $\mathcal{A} = M_2(\mathbb{C})$ .

This reconstruction procedure may be generalized to arbitrary  $C^*$ -algebras [Landsman, 1998], and defines the precise connection between the Schrödinger picture and the Heisenberg picture that is relevant to decoherence. These pictures are equivalent, but in practice the reconstruction procedure may be difficult to carry through.

11. For this reason it is of interest to have a direct description of decoherence in the Heisenberg picture. Such a description has been developed by Blanchard and Olkiewicz [2003], partly on the basis of earlier results by Olkiewicz [1999a,b; 2000]. Mathematically, their approach is more powerful than the Schrödinger picture on which most of the literature on decoherence is based. Let  $\mathcal{A}_S = \mathcal{B}(\mathcal{H}_S)$  and  $\mathcal{A}_E = \mathcal{B}(\mathcal{H}_E)$ , and assume one has a total Hamiltonian  $H$  acting on  $\mathcal{H}_S \otimes \mathcal{H}_E$  as well as a fixed state of the environment, represented by a density matrix  $\rho_E$  (often taken to be a thermal equilibrium state). If  $\rho_S$  is a density matrix on  $\mathcal{H}_S$  (so that the total state is  $\rho_S \otimes \rho_E$ ), the Schrödinger

picture approach to decoherence (and more generally to the quantum theory of open systems) is based on the time-evolution

$$(1) \quad \rho_S(t) = \text{Tr}_{\mathcal{H}_E} \left( e^{-\frac{it}{\hbar}H} \rho_S \otimes \rho_E e^{\frac{it}{\hbar}H} \right).$$

The Heisenberg picture, on the other hand, is based on the associated operator time-evolution for  $A \in \mathcal{B}(\mathcal{H}_S)$  given by

$$(2) \quad A(t) = \text{Tr}_{\mathcal{H}_E} \left( \rho_E e^{\frac{it}{\hbar}H} A \otimes 1 e^{-\frac{it}{\hbar}H} \right),$$

since this yields the equivalence of the Schrödinger and Heisenberg pictures expressed by

$$(3) \quad \text{Tr}_{\mathcal{H}_S} (\rho_S(t)A) = \text{Tr}_{\mathcal{H}_S} (\rho_S A(t)).$$

More generally, let  $\mathcal{A}_S$  and  $\mathcal{A}_E$  be unital  $C^*$ -algebras with spatial tensor product  $\mathcal{A}_S \otimes \mathcal{A}_E$ , equipped with a time-evolution  $\alpha_t$  and a fixed state  $\omega_E$  on  $\mathcal{A}_E$ . This defines a conditional expectation  $P_E : \mathcal{A}_S \otimes \mathcal{A}_E \rightarrow \mathcal{A}_S$  by linear and continuous extension of  $P_E(A \otimes B) = A\omega_E(B)$ , and consequently a reduced time-evolution  $A \mapsto A(t)$  on  $\mathcal{A}_S$  via

$$(4) \quad A(t) = P_E(\alpha_t(A \otimes 1)).$$

See, for example, Alicki and Lendi [1987]; in our context, this generality is crucial for the potential emergence of continuous classical phase spaces; see below.<sup>319</sup> Now the key point is that decoherence is described by a decomposition  $\mathcal{A}_S = \mathcal{A}_S^{(1)} \oplus \mathcal{A}_S^{(2)}$  as a vector space (not as a  $C^*$ -algebra), where  $\mathcal{A}_S^{(1)}$  is a  $C^*$ -algebra, with the property that  $\lim_{t \rightarrow \infty} A(t) = 0$  (weakly) for all  $A \in \mathcal{A}_S^{(2)}$ , whereas  $A \mapsto A(t)$  is an automorphism on  $\mathcal{A}_S^{(1)}$  for each finite  $t$ . Consequently,  $\mathcal{A}_S^{(1)}$  is the effective algebra of observables after decoherence, and it is precisely the pure states on  $\mathcal{A}_S^{(1)}$  that are robust or einselected in the sense discussed before.

12. For example, if  $\mathcal{A}_S = M_2(\mathbb{C})$  and the states  $\uparrow$  and  $\downarrow$  are robust under decoherence, then  $\mathcal{A}_S^{(1)} = \mathbb{C} \oplus \mathbb{C}$  and  $\mathcal{A}_S^{(2)}$  consists of all  $2 \times 2$  matrices with zeros on the diagonal. In this example  $\mathcal{A}_S^{(1)}$  is commutative hence classical, but this may not be the case in general. But if it is, the automorphic time-evolution on  $\mathcal{A}_S^{(1)}$  induces a classical flow on its structure space, which should be shown to be Hamiltonian using the techniques of Section 6.<sup>320</sup>

<sup>319</sup>For technical reasons Blanchard and Olkiewicz [2003] assume  $\mathcal{A}_S$  to be a von Neumann algebra with trivial center.

<sup>320</sup>Since on the assumption in the preceding footnote  $\mathcal{A}_S^{(1)}$  is a commutative von Neumann algebra one should define the structure space in an indirect way; see [Blanchard and Olkiewicz, 2003].

In any case, there will be some sort of classical behaviour of the decohered system whenever  $\mathcal{A}_S^{(1)}$  has a nontrivial center.<sup>321</sup> If this center is discrete, then the induced time-evolution on it is necessarily trivial, and one has the typical measurement situation where the center in question is generated by the projections on the eigenstates of a pointer observable with discrete spectrum. This is generic for the case where  $\mathcal{A}_S$  is a type I factor. However, type II and III factors may give rise to continuous classical systems with nontrivial time-evolution; see [Lugiewicz and Olkiewicz, 2002; 2003]. We cannot do justice here to the full technical details and complications involved here. But we would like to emphasize that further to quantum field theory and the theory of the thermodynamic limit, the present context of decoherence should provide important motivation for specialists in the foundations of quantum theory to learn the theory of operator algebras.<sup>322</sup>

## 7.2 Consistent histories

Whilst doing so, one is well advised to work even harder and simultaneously familiarize oneself with *consistent histories*. This approach to quantum theory was pioneered by Griffiths [1984] and was subsequently taken up by Omnès [1992] and others. Independently, Gell-Mann and Hartle [1990; 1993] proposed analogous ideas. Like decoherence, the consistent histories method has been the subject of lengthy reviews [Hartle, 1995] and even books [Omnès, 1994; 1999; Griffiths, 2002] by the founders. See also the reviews by Kiefer [2003] and Halliwell [2004], the critiques by Dowker and Kent [1996], Kent [1998], Bub [1999], and Bassi and Ghirardi [2000], as well as the various mathematical reformulations and reinterpretations of the consistent histories program [Isham, 1994; 1997; Isham and Linden, 1994; 1995; Isham *et al.*, 1994; Isham and Butterfield, 2000; Rudolph, 1996a; 1996b; 2000; Rudolph and Wright, 1999].

The relationship between consistent histories and decoherence is somewhat peculiar: on the one hand, decoherence is a natural mechanism through which appropriate sets of histories become (approximately) consistent, but on the other hand these approaches appear to have quite different points of departure. Namely, where decoherence starts from the idea that (quantum) systems are naturally coupled to their environments and therefore have to be treated as *open* systems, the aim of consistent histories is to deal with *closed* quantum systems such as the Universe, without a priori talking about measurements or observers. However, this distinction is merely historical: as we have seen in item 6 in the previous subsection, the dividing line between a system and its environment should be seen as a dynamical entity to be drawn according to certain stability criteria, so that even in decoherence theory one should really study the system plus its environment as a whole from the outset.<sup>323</sup> And this is precisely what consistent historians do.

<sup>321</sup>This is possible even when  $\mathcal{A}_S$  is a factor!

<sup>322</sup>See the references in footnote 7.

<sup>323</sup>This renders the distinction between “open” and “closed” systems a bit of a red herring, as

As in the preceding subsection, and for exactly the same reasons, we format our treatment of consistent histories as a list of items open to discussion.

1. The starting point of the consistent histories formulation of quantum theory is conventional: one has a Hilbert space  $\mathcal{H}$ , a state  $\rho$ , taken to be the initial state of the total system under consideration (realized as a density matrix on  $\mathcal{H}$ ) and a Hamiltonian  $H$  (defined as a self-adjoint operator on  $\mathcal{H}$ ). What is unconventional is that this total system may well be the entire Universe. Each property  $\alpha$  of the total system is mathematically represented by a projection  $P_\alpha$  on  $\mathcal{H}$ ; for example, if  $\alpha$  is the property that the energy takes some value  $\epsilon$ , then the operator  $P_\alpha$  is the projection onto the associated eigenspace (assuming  $\epsilon$  belongs to the discrete spectrum of  $H$ ). In the Heisenberg picture,  $P_\alpha$  evolves in time as  $P_\alpha(t)$  according to (12); note that  $P_\alpha(t)$  is once again a projection.

A *history*  $\mathbb{H}_A$  is a chain of properties (or propositions)  $(\alpha_1(t_1), \dots, \alpha_n(t_n))$  indexed by  $n$  different times  $t_1 < \dots < t_n$ ; here  $A$  is a multi-label incorporating both the properties  $(\alpha_1, \dots, \alpha_n)$  and the times  $(t_1, \dots, t_n)$ . Such a history indicates that each property  $\alpha_i$  holds at time  $t_i$ ,  $i = 1, \dots, n$ . Such a history may be taken to be a collection  $\{\alpha(t)\}_{t \in \mathbb{R}}$  defined for all times, but for simplicity one usually assumes that  $\alpha(t) \neq 1$  (where 1 is the trivial property that always holds) only for a finite set of times  $t$ ; this set is precisely  $\{t_1, \dots, t_n\}$ . An example suggested by Heisenberg (1927) is to take  $\alpha_i$  to be the property that a particle moving through a Wilson cloud chamber may be found in a cell  $\Delta_i \subset \mathbb{R}^6$  of its phase space; the history  $(\alpha_1(t_1), \dots, \alpha_n(t_n))$  then denotes the state of affairs in which the particle is in cell  $\Delta_1$  at time  $t_1$ , subsequently is in cell  $\Delta_2$  at time  $t_2$ , etcetera. Nothing is stated about the particle's behaviour at intermediate times. Another example of a history is provided by the double slit experiment, where  $\alpha_1$  is the particle's launch at the source at  $t_1$  (which is usually omitted from the description),  $\alpha_2$  is the particle passing through (e.g.) the upper slit at  $t_2$ , and  $\alpha_3$  is the detection of the particle at some location  $L$  at the screen at  $t_3$ . As we all know, there is a potential problem with this history, which will be clarified below in the present framework.

The fundamental claim of the consistent historians seems to be that quantum theory should do no more (or less) than making predictions about the probabilities that histories occur. What these probabilities actually mean remains obscure (except perhaps when they are close to zero or one, or when reference is made to some measurement context; see [Hartle, 2005]), but let us first see when and how one can define them. The only potentially meaningful mathematical expression (within quantum mechanics) for the probability of

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even in decoherence theory the totality of the system plus its environment is treated as a closed system.

a history  $\mathbb{H}_A$  with respect to a state  $\rho$  is [Groenewold, 1952; Wigner, 1963]

$$(5) \quad p(\mathbb{H}_A) = \text{Tr}(C_A \rho C_A^*),$$

where

$$(6) \quad C_A = P_{\alpha_n}(t_n) \cdots P_{\alpha_1}(t_1).$$

Note that  $C_A$  is generally not a projection (and hence a property) itself (unless all  $P_{\alpha_i}$  mutually commute). In particular, when  $\rho = [\Psi]$  is a pure state (defined by some unit vector  $\Psi \in \mathcal{H}$ ), one simply has

$$(7) \quad p(\mathbb{H}_A) = \|C_A \Psi\|^2 = \|P_{\alpha_n}(t_n) \cdots P_{\alpha_1}(t_1) \Psi\|^2.$$

When  $n = 1$  this just yields the Born rule. Conversely, see Isham (1994) for a derivation of (5) from the Born rule.<sup>324</sup>

2. Whatever one might think about the metaphysics of quantum mechanics, a probability makes no sense whatsoever when it is only attributed to a single history (except when it is exactly zero or one). The least one should have is something like a sample space (or event space) of histories, each (measurable) subset of which is assigned some probability such that the usual (Kolmogorov) rules are satisfied. This is a (well-known) problem even for a single time  $t$  and a single projection  $P_\alpha$  (i.e.  $n = 1$ ). In that case, the problem is solved by finding a self-adjoint operator  $A$  of which  $P_\alpha$  is a spectral projection, so that the sample space is taken to be the spectrum  $\sigma(A)$  of  $A$ , with  $\alpha \subset \sigma(A)$ . Given  $P_\alpha$ , the choice of  $A$  is by no means unique, of course; different choices may lead to different and incompatible sample spaces. In practice, one usually starts from  $A$  and derives the  $P_\alpha$  as its spectral projections  $P_\alpha = \int_\alpha dP(\lambda)$ , given that the spectral resolution of  $A$  is  $A = \int_{\mathbb{R}} dP(\lambda) \lambda$ . Subsequently, one may then either *coarse-grain* or *fine-grain* this sample space. The former is done by finding a partition  $\sigma(A) = \coprod_i \alpha_i$  (disjoint union), and only admitting elements of the  $\sigma$ -algebra generated by the  $\alpha_i$  as events (along with the associated spectral projection  $P_{\alpha_i}$ ), instead of all (measurable) subsets of  $\sigma(A)$ . To perform fine-graining, one supplements  $A$  by operators that commute with  $A$  as well as with each other, so that the new sample space is the joint spectrum of the ensuing family of mutually commuting operators.

In any case, in what follows it turns out to be convenient to work with the projections  $P_\alpha$  instead of the subsets  $\alpha$  of the sample space; the above discussion then amounts to extending the given projection on  $\mathcal{H}$  to some

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<sup>324</sup>See also [Zurek, 2005] for a novel derivation of the Born rule, as well as the ensuing discussion in [Schlosshauer, 2004].

Boolean sublattice of the lattice  $\mathcal{P}(\mathcal{H})$  of all projections on  $\mathcal{H}$ .<sup>325</sup> Any state  $\rho$  then defines a probability measure on this sublattice in the usual way [Beltrametti and Cassinelli, 1984].

3. Generalizing this to the multi-time case is not a trivial task, somewhat facilitated by the following device (Isham, 1994). Put  $\mathcal{H}^N = \otimes^N \mathcal{H}$ , where  $N$  is the cardinality of the set of all times  $t_i$  relevant to the histories in the given collection,<sup>326</sup> and, for a given history  $\mathbb{H}_A$ , define

$$(8) \quad \mathbb{C}_A = P_{\alpha_n}(t_n) \otimes \cdots \otimes P_{\alpha_1}(t_1).$$

Here  $P_{\alpha_i}(t_i)$  acts on the copy of  $\mathcal{H}$  in the tensor product  $\mathcal{H}^N$  labeled by  $t_i$ , so to speak. Note that  $\mathbb{C}_A$  is a projection on  $\mathcal{H}^N$  (whereas  $C_A$  in (6) is generally *not* a projection on  $\mathcal{H}$ ). Furthermore, given a density matrix  $\rho$  on  $\mathcal{H}$  as above, define the *decoherence functional*  $d$  as a map from pairs of histories into  $\mathbb{C}$  by

$$(9) \quad d(\mathbb{H}_A, \mathbb{H}_B) = \text{Tr}(C_A \rho C_B^*).$$

The main point of the consistent histories approach may now be summarized as follows: a collection  $\{\mathbb{H}_A\}_{A \in \mathbb{A}}$  of histories can be regarded as a sample space on which a state  $\rho$  defines a probability measure via (5), which of course amounts to

$$(10) \quad p(\mathbb{H}_A) = d(\mathbb{H}_A, \mathbb{H}_A),$$

provided that:

- (a) The operators  $\{\mathbb{C}_A\}_{A \in \mathbb{A}}$  form a Boolean sublattice of the lattice  $\mathcal{P}(\mathcal{H}^N)$  of all projections on  $\mathcal{H}^N$ ;
- (b) The real part of  $d(\mathbb{H}_A, \mathbb{H}_B)$  vanishes whenever  $\mathbb{H}_A$  is disjoint from  $\mathbb{H}_B$ .<sup>327</sup>

In that case, the set  $\{\mathbb{H}_A\}_{A \in \mathbb{A}}$  is called *consistent*. It is important to realize that the possible consistency of a given set of histories depends (trivially) not only on this set, but in addition on the dynamics and on the initial state.

Consistent sets of histories generalize families of commuting projections at a single time. There is no great loss in replacing the second condition by the vanishing of  $d(\mathbb{H}_A, \mathbb{H}_B)$  itself, in which case the histories  $\mathbb{H}_A$  and  $\mathbb{H}_B$  are

<sup>325</sup>This sublattice is supposed to the unit of  $\mathcal{P}(\mathcal{H})$ , i.e. the unit operator on  $\mathcal{H}$ , as well as the zero projection. This comment also applies to the Boolean sublattice of  $\mathcal{P}(\mathcal{H}^N)$  discussed below.

<sup>326</sup>See the mathematical references above for the case  $N = \infty$ .

<sup>327</sup>This means that  $\mathbb{C}_A \mathbb{C}_B = 0$ ; equivalently,  $P_{\alpha_i}(t_i) P_{\beta_i}(t_i) = 0$  for at least one time  $t_i$ . This condition guarantees that the probability (10) is additive on disjoint histories.

said to *decohere*.<sup>328</sup> For example, in the double slit experiment the pair of histories  $\{\mathbb{H}_A, \mathbb{H}_B\}$  where  $\alpha_1 = \beta_1$  is the particle's launch at the source at  $t_1$ ,  $\alpha_2$  ( $\beta_2$ ) is the particle passing through the upper (lower) slit at  $t_2$ , and  $\alpha_3 = \beta_3$  is the detection of the particle at some location  $L$  at the screen, is *not consistent*. It becomes consistent, however, when the particle's passage through either one of the slits is recorded (or measured) *without the recording device being included in the histories* (if it is, nothing would be gained). This is reminiscent of the von Neumann chain in quantum measurement theory, which indeed provides an abstract setting for decoherence (cf. item 1 in the preceding subsection). Alternatively, the set can be made consistent by omitting  $\alpha_2$  and  $\beta_2$ . See [Griffiths, 2002] for a more extensive discussion of the double slit experiment in the language of consistent histories.

More generally, coarse-graining by simply leaving out certain properties is often a promising attempt to make a given inconsistent set consistent; if the original history was already consistent, it can never become inconsistent by doing so. Fine-graining (by embedding into a larger set), on the other hand, is a dangerous act in that it may render a consistent set inconsistent.

4. What does it all mean? Each choice of a consistent set defines a “universe of discourse” within which one can apply classical probability theory and classical logic [Omnès, 1992]. In this sense the consistent historians are quite faithful to the Copenhagen spirit (as most of them acknowledge): *in order to understand it, the quantum world has to be looked at through classical glasses*. In our opinion, no convincing case has ever been made for the absolute necessity of this Bohrian stance (cf. Subsection 3.1), but accepting it, the consistent histories approach is superior to Copenhagen in not relying on measurement as an a priori ingredient in the interpretation of quantum mechanics.<sup>329</sup> It is also more powerful than the decoherence approach in turning the notion of a system into a dynamical variable: different consistent sets describe different systems (and hence different environments, defined as the rest of the Universe); cf. item 6 in the previous subsection.<sup>330</sup> In other words, the choice of a consistent set boils down to a choice of “relevant variables” against “irrelevant” ones omitted from the description. As indeed

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<sup>328</sup>Consistent historians use this terminology in a different way from decoherence theorists. By definition, any two histories involving only a single time are consistent (or, indeed, “decohere”) iff condition (a) above holds; condition (b) is trivially satisfied in that case, and becomes relevant only when more than one time is considered. However, in decoherence theory the reduced density matrix at some given time does not trivially “decohere” at all; the whole point of the (original) decoherence program was to provide models in which this happens (if only approximately) because of the coupling of the system with its environment. Having said this, within the context of models there are close links between consistency (or decoherence) of multi-time histories and decoherence of reduced density matrices, as the former is often (approximately) achieved by the same kind of dynamical mechanisms that lead to the latter.

<sup>329</sup>See [Hartle, 2005] for an analysis of the connection between consistent histories and the Copenhagen interpretation and others.

<sup>330</sup>Technically, as the commutant of the projections occurring in a given history.

stressed in the literature, the act of identification of a certain consistent set as a universe of discourse is itself nothing but a coarse-graining of the Universe as a whole.

5. But these conceptual successes come with a price tag. Firstly, *consistent sets turn out not to exist in realistic models* (at least if the histories in the set carry more than one time variable). This has been recognized from the beginning of the program, the response being that one has to deal with approximately consistent sets for which (the real part of)  $d(\mathbb{H}_A, \mathbb{H}_B)$  is merely very small. Furthermore, even the definition of a history often cannot be given in terms of projections. For example, in Heisenberg's cloud chamber example (see item 1 above), because of his very own uncertainty principle it is impossible to write down the corresponding projections  $P_{\alpha_i}$ . A natural candidate would be  $P_\alpha = Q_h^B(\chi_\Delta)$ , cf. (19) and (28), but in view of (21) this operator fails to satisfy  $P_\alpha^2 = P_\alpha$ , so that it is not a projection (although it does satisfy the second defining property of a projection  $P_\alpha^* = P_\alpha$ ). This merely reflects the usual property  $Q(f)^2 \neq Q(f^2)$  of any quantization method, and necessitates the use of approximate projections [Omnès, 1997]. Indeed, this point calls for a reformulation of the entire consistent histories approach in terms of positive operators instead of projections [Rudolph, 1996a,b].

These are probably not serious problems; indeed, the recognition that classicality emerges from quantum theory only in an approximate sense (conceptually as well as mathematically) is a profound one (see the Introduction), and it rather should be counted among its blessings that the consistent histories program has so far confirmed it.

6. What is potentially more troubling is that consistency by no means implies classicality *beyond the ability (within a given consistent set) to assign classical probabilities and to use classical logic*. Quite to the contrary, neither Schrödinger cat states nor histories that look classical at each time but follow utterly unclassical trajectories in time are forbidden by the consistency conditions alone [Dowker and Kent, 1996]. But is this a genuine problem, except to those who still believe that the earth is at the centre of the Universe and/or that humans are privileged observers? It just seems to be the case that — at least according to the consistent historians — the ontological landscape laid out by quantum theory is far more “inhuman” (or some would say “obscure”) than the one we inherited from Bohr, in the sense that most consistent sets bear no obvious relationship to the world that *we* observe. In attempting to make sense of these, no appeal to “complementarity” will do now: for one, the complementary pictures of the quantum world called for by Bohr were classical in a much stronger sense than generic consistent sets are, and on top of that Bohr asked us to only think about two such pictures, as opposed to the innumerable consistent sets offered to us. Our conclusion is that, much as decoherence does not solve the measurement problem but rather aggravates it (see item 2 in the preceding subsection), also *consistent*



*histories actually make the problem of interpreting quantum mechanics more difficult than it was thought to be before.* In any case, it is beyond doubt that the consistent historians have significantly deepened our understanding of quantum theory — at the very least by providing a good bookkeeping device!

7. Considerable progress has been made in the task of identifying at least *some* (approximately) consistent sets that display (approximate) classical behaviour in the full sense of the word [Gell-Mann and Hartle, 1993; Omnès, 1992; 1997; Halliwell, 1998; 2000; 2004; Brun and Hartle, 1999; Bosse and Hartle, 2005]. Indeed, in our opinion studies of this type form the main concrete outcome of the consistent histories program. The idea is to find a consistent set  $\{\mathbb{H}_A\}_{A \in \mathbb{A}}$  with three decisive properties:

- (a) Its elements (i.e. histories) are strings of propositions with a classical interpretation;
- (b) Any history in the set that delineates a classical trajectory (i.e. a solution of appropriate classical equations of motion) has probability (10) close to unity, and any history following a classically impossible trajectory has probability close to zero;
- (c) The description is sufficiently coarse-grained to achieve consistency, but is sufficiently fine-grained to turn the deterministic equations of motion following from (b) into a closed system.

When these goals are met, it is in this sense (no more, no less) that the consistent histories program can claim with some justification that it has indicated (or even explained) ‘How the quantum Universe becomes classical’ [Halliwell, 2005].

Examples of propositions with a classical interpretation are quantized classical observables with a recognizable interpretation (such as the operators  $Q_{\hbar}^B(\chi_{\Delta})$  mentioned in item 5), macroscopic observables of the kind studied in Subsection 6.1, and hydrodynamic variables (i.e. spatial integrals over conserved currents). These represent three different levels of classicality, which in principle are connected through mutual fine- or coarse-grainings.<sup>331</sup> The first are sufficiently coarse-grained to achieve consistency only in the limit  $\hbar \rightarrow 0$  (cf. Section 5), whereas the latter two are already coarse-grained by their very nature. Even so, also the initial state will have to be “classical” in some sense in order to achieve the three targets (a) - (c).

All this is quite impressive, but we would like to state our opinion that neither decoherence nor consistent histories can stand on their own in explaining the appearance of the classical world. Promising as these approaches are, they have to

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<sup>331</sup>The study of these connections is relevant to the program laid out in this paper, but really belongs to classical physics *per se*; think of the derivation of the Navier–Stokes equations from Newton’s equations.

be combined at least with limiting techniques of the type described in Sections 5 and 6 — not to speak of the need for a new metaphysics! For even if it is granted that decoherence yields the disappearance of superpositions of Schrödinger cat type, or that consistent historians give us consistent sets none of whose elements contain such superpositions among their properties, this by no means suffices to explain the emergence of classical phase spaces and flows thereon determined by classical equations of motion. Since so far the approaches cited in Sections 5 and 6 have hardly been combined with the decoherence and/or the consistent histories program, a full explanation of the classical world from quantum theory is still in its infancy. This is not merely true at the technical level, but also conceptually; what has been done so far only represents a modest beginning. On the positive side, here lies an attractive challenge for mathematically minded researchers in the foundations of physics!

## 8 EPILOGUE

As a sobering closing note, one should not forget that whatever one's achievements in identifying a "classical realm" in quantum mechanics, the theory continues to incorporate another realm, the pure quantum world, that the young Heisenberg first gained access to, if not through his mathematics, then perhaps through the music of his favourite composer, Beethoven. This world beyond ken has never been better described than by Hoffmann [1810] in his essay on Beethoven's instrumental music, and we find it appropriate to end this paper by quoting at some length from it.<sup>332</sup>

Should one, whenever music is discussed as an independent art, not always be referred to instrumental music which, refusing the help of any other art (of poetry), expresses the unique essence of art that can only be recognized in it? It is the most romantic of all arts, one would almost want to say, the only truly romantic one, for only the infinite is its source. Orpheus' lyre opened the gates of the underworld. Music opens to man an unknown realm, a world that has nothing in common with the outer sensual world that surrounds him, a realm in which he leaves behind all of his feelings of certainty, in order to abandon himself to an unspeakable longing. (...)

Beethoven's instrumental music opens to us the realm of the gigantic and unfathomable. Glowing rays of light shoot through the dark night of this realm, and we see gigantic shadows swaying back and forth, encircling us closer and closer, destroying us (...) Beethoven's music moves the levers of fear, of shudder, of horror, of pain and thus awakens that infinite longing that is the essence of romanticism. Therefore, he is a purely romantic composer, and may it not be because of it, that

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<sup>332</sup>Translation copyright: Ingrid Schwaegermann [2001].

to him, vocal music that does not allow for the character of infinite longing — but, through words, achieves certain effects, as they are not present in the realm of the infinite — is harder?(...)

What instrumental work of Beethoven confirms this to a higher degree than his magnificent and profound Symphony in c-Minor. Irresistibly, this wonderful composition leads its listeners in an increasing climax towards the realm of the spirits and the infinite.(...) Only that composer truly penetrates into the secrets of harmony who is able to have an effect on human emotions through them; to him, relationships of numbers, which, to the Grammarian, must remain dead and stiff mathematical examples without genius, are magic potions from which he lets a miraculous world emerge. (...)

Instrumental music, wherever it wants to only work through itself and not perhaps for a certain dramatic purpose, has to avoid all unimportant punning, all dallying. It seeks out the deep mind for premonitions of joy that, more beautiful and wonderful than those of this limited world, have come to us from an unknown country, and spark an inner, wonderful flame in our chests, a higher expression than mere words — that are only of this earth — can spark.

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