university of groningen

Bohmian insights into mathematical scattering theory

Bachelor Thesis

BSc Physics and BSc Mathematics
Faculty of Science and Engineering
University of Groningen
July 30, 2021

Author:
Vladimir Ioan Rotariu

First supervisor:
dr. Marcello Seri

Second supervisor:
Prof. dr. Diederik Roest

Contents

Introduction

The measurement problem is arguably the thorniest issue of the orthodox interpretation of quantum mechanics (OQM). It has to do with establishing the existence and mechanism of the wave function collapse under an observation: we are often introduced to it by way of *Schrödinger's cat*, a thought experiment that entered pop culture a long time ago.

Nevertheless, it is all too easy to slap a Schrödinger's cat-inspired logo on a T-shirt and forget that the measurement problem is at the heart of a (bloodless) guerrilla war in modern physics: the dissatisfaction with OQM led to interpretations where the wave function collapse is absent, such as Bohmian mechanics (BM) [Boh52] and the many-worlds interpretation [Eve57], or where the collapse is governed by a stochastic process, such as the one in [GRW86], to name just a few of the options listed in the survey about the 'foundational attitudes toward quantum mechanics' discussed in [SKZ13].

There is, however, a surprising undertone to the findings presented in [SKZ13]: the majority of the physicists, philosophers and mathematicians that provided answers to the survey agreed that their choice of interpretation of quantum mechanics is 'a matter of personal philosophical prejudice', i.e. given different interpretations that agree with the experiments, one would often choose one for rather subjective reasons. This prompts us to wonder: all is well, but what happens with the measurement problem? 24% of the same cohort of intellectuals considered it 'a severe difficulty threatening quantum mechanics', while the others are, for various reasons, not bothered by it.

In this work, we will identify ourselves with the 24% of disquieted scientists and consider BM's take on modelling the scattering of a single nonrelativistic spinless particle, owing to the absence of wave collapse in BM (see [Mau95]). We are going to first discuss OQM in general, deriving its principles from general assumptions. Then, in Section 2 we introduce the reader to orthodox mathematical scattering theory, where a central topic are the so-called 'Möller wave operators', which roughly speaking allow us to classify the states of our quantum system in 'bound states' and 'scattering states', and are connected directly to the experimentally relevant 'orthodox scattering cross section'. In Section 3, we provide a derivation of the equations of BM by means of symmetry requirements; we contrast this new theory with OQM, but we also stress the reconciliation between Heisenberg's uncertainty principle and the fact that the particles in BM have definite (random) positions. And finally, the Bohmian insights into mathematical scattering theory are reserved for Section 4: we will prove that the 'Bohmian scattering cross section' and the 'orthodox scattering cross section' are equal, and we will devise a Bohmian sufficient condition to identify a 'scattering state'.

On notation and units: In this work we will set the reduced Planck constant $\hbar = 1$, and also the mass of the particle will be taken to be $m = 1/2$, such that the free Hamiltonian is equal to the Laplacian operator (exceptions from the $m = 1/2$ rule are Subsection 1.1, 1.4, 1.5, while exceptions from both are Subsection 3.2 and 3.3).

We will exclusively refer to '$\langle \cdot, \cdot \rangle$' for the natural inner product of $L^2(\mathbb{R}^m)$, for an $m \geq 1$ that will be clear from the context[1], and similarly we will use '$\| \cdot \|$' for the norm induced by the natural inner product of $L^2(\mathbb{R}^m)$.

[1] I.e. in Section 1 our particle lives on (subsets of) $\mathbb{R}$ to facilitate the derivations, in Sections 2 and 4 we are working in $\mathbb{R}^m$ as there are no reasons not to be general, while in Section 3 the particle is in $\mathbb{R}^3$ as we are interested in being as close as possible to a real scattering setup when deriving BM.

1. The rudiments of orthodox quantum mechanics on firm mathematical grounds

The purpose of this section is twofold: on one hand, we aim to present the main principles of orthodox quantum mechanics (OQM) guised under the so-called 'axioms of OQM', while on the other hand the mathematics underpinning the latter will be introduced.

Disclaimer: while we strived to write this section in a self-contained manner, we assumed a certain degree of familiarity with elementary OQM, measure theory, and functional analysis. We kindly refer the reader to the classical textbook [SN11] for the physical concepts that are used in this section, while more rigorous treatments that include the necessary mathematical notions can be found in [Tes14] and [Hal13]. In fact, the core of this section is based on exactly the aforementioned three references.

1.1. Beyond the classical realm

Suppose we have a particle of mass m attached to the end of a spring with stiffness k; we stretch the spring, and then release it, thus obtaining a so-called *harmonic oscillator*.

We can model the harmonic oscillator using classical mechanics (CM). The dynamics[2] in CM is given by *Hamilton's equations*:

$$\frac{dx}{dt} = \{x, H_{\text{cl}}\}\,, \quad \frac{dp}{dt} = \{p, H_{\text{cl}}\}\,, \tag{1}$$

where

$$\{f, g\} \coloneqq \frac{\partial f}{\partial x}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial x}$$

is the *Poisson bracket*, and the *total energy function* H_{cl} commonly assumes the form

$$H_{\text{cl}}(x, p) \coloneqq \frac{1}{2m}p^2 + V(x),$$

where the first term represents the *kinetic energy*, and V is the *potential energy function* as specified by the classical system[3] we are modelling (see [DT09, p.13-p.23] for a concise introduction to the Hamiltonian formulation of classical mechanics).

Hamilton's equations imply that all we need to know about the particle that oscillates attached to a spring is represented by its position x and momentum p. However, in order to solve (1) for x and p, we need to know the specific H_{cl} of the harmonic oscillator. We

[2]In anticipation of Subsection 1.5, we prefer to model the dynamics of our physical system using the Hamiltonian formulation of classical mechanics.

[3]From now we will often refer to a physical system modelled using CM/OQM as the 'classical system'/'quantum system'.

first relabel it as 'E_{cl}' to avoid confusion in the future, and then we remember that CM predicts that the total energy of the harmonic oscillator is given by

$$E_{\text{cl}}(x,p) = \frac{1}{2m}p^2 + \frac{k}{2}x^2. \tag{2}$$

We know from experimental practice that the energy is an empirical quantity[4]; based on the expression above, we further see that E_{cl} is a function of the two primal variables[5] of CM. We call such a mapping a *CM observable*[6], as it links (some of) the variables of the theory (in our case empirical quantities as well, the primal variables x and p) with a **real** scalar that can be empirically determined (namely E_{cl}, the total energy of the classical harmonic oscillator).

Back to the particle attached to the end of a spring. When considering (2), the question follows: do we have any forbidden energies? As long as we pose no restrictions on what x and p our particle may assume, (2) blatantly implies that we can have any $E_{\text{cl}} \in \mathbb{R}_0^+$, thus a **continuous** 'energy spectrum'.

The classical harmonic oscillator seems like a good model for vibrating molecules. However, many experiments do attest the fact that the total energy of a vibrating molecule **cannot** assume any value in $\mathbb{R}_0^+$[AdP06]; indeed, at such a small scale, the so-called 'quantum effects', i.e. deviations from the predictions of CM, do manifest. OQM's goal is to take note of these deviating effects[7] and provide us with a solid theory whenever CM fails to correctly describe the Nature. It instructs us to model our system in the following way: whereas in CM we have the position x and momentum p (obtained from Hamilton's equations) that provides us with a full description, in OQM we have a function ψ (a solution of the time-dependent Schrödinger equation (39)) with an identical purpose[8]; consequently, the total energy of the quantum system is now obtained by acting with the *self-adjoint operator*

$$E_{\text{qt}} := \frac{1}{2m}P^2 + \frac{k}{2}X^2 \tag{3}$$

on the states $\{\psi_i\}_{n=1}^{\infty}$ which are its eigenfunctions[9]

$$E_{\text{qt}}\psi = \lambda_E \psi; \tag{4}$$

[4]Viz. that can be measured in an experiment.

[5]The variables that a given theory is about.

[6]The reader should consider this a rule of thumb; for a rigorous definition, see [FM06].

[7]In this work we completely **ignore** any relativistic effect.

[8]At first glance it seems controversial to put x&p and ψ on the same par, and not, say, by replacing the latter with quantities that can be readily identified as having the meaning of position and momentum, but the reader should be aware of the fact that the primal variables of a theory are **not** necessarily the ones that have the property of being empirical, but rather the ones appearing in its construction (e.g. first principles); in the case of CM, the fact that the primal variables are also empirical is just a (fortunate, but also confusing) coincidence.

[9]We did not include here the expressions for the eigenfunctions that can be obtained from (4)(see

we interpret the real eigenvalues[10] λ_E as the total energy, for a given X and P defined in such a way that they bear an analogous meaning[11] in OQM to x and p in CM.

Here comes the discord with OQM: for the quantum harmonic oscillator, the eigenvalues (read 'the allowed energies') cannot take any value in $\mathbb{R}_0^+$, as it was the case in CM, but rather are of the form:

$$\lambda_{E,n} = \left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}},\ \text{with } n \in \mathbb{N}_0; \tag{5}$$

(the explicit calculations can be found in [SN11, p.89-p.94]).

There are many things 'wrong' with the equation above, from the point of view of CM. In the first place, we repeat that we do not have a 'continuum' of possible energies (in the case of the harmonic oscillator, $\mathbb{R}_0^+$); instead, we are restricted to an infinity of **discrete** values. And secondly, the *ground state* (the state with the lowest value of energy) is not of zero energy, but is stuck at a fixed positive value $\lambda_{E,0}$. We will take care of pointing to other dissimilarities between OQM and CM along the way; for now, it is worth bearing in mind that E_{qt} is an example of an *OQM observable*: it is acting on the primal variable of the theory, ψ, and, in the case that the latter is its eigenfunction, the ensuing eigenvalue is a real number which can be interpreted as the total energy of the system under consideration. Although the route from observables to empirical quantities seems in the quantum regime a little bit more cumbersome than in the classical one (solving an eigenequation versus evaluating a function), (2) and (4) have identical meaning in their respective theories.

We said that (3) represents a self-adjoint operator, but on what exactly does it act, i.e. what is its domain $\mathfrak{D}(E_{\text{qt}})$? As we used X^2 and P^2 in its definition, the more precise question would be to ask for explicit $\mathfrak{D}(X^2)$ and $\mathfrak{D}(P^2)$. We collect the ψ relevant for the harmonic oscillator in a set[12] $\mathfrak{H}$, and we take for simplicity $\mathfrak{D}(E_{\text{qt}}) = \mathfrak{D}(X^2) \cap \mathfrak{D}(P^2)$; if one wishes to define e.g. $\mathfrak{D}(X^2)$ without any extra information from our physical setup, then a natural choice would be to first define

$$\mathfrak{D}(X) := \{\psi \in \mathfrak{H} : X\psi \in \mathfrak{H}\},$$

and then, similarly,

$$\mathfrak{D}(X^2) := \{\psi \in \mathfrak{D}(X) : X\psi \in \mathfrak{H}\}.$$

[Hal13, p.232] for their derivation using the 'analytical method' of solving the quantum harmonic oscillator); however, one might solve the quantum harmonic oscillator using Dirac's 'algebraic method', which starts only with (33) as an assumption (see [Hal13, p.288-232]) for Dirac's clever trick).

[10]See the first part of Appendix A.

[11]We will return to this point in the next subsection (Axiom 2).

[12]Based on, say, (4), a general OQM observable A is defined in such a way that its range $\mathfrak{R}(A)$ is included in $\mathfrak{H}$.

But what exactly are X and P? If they would act on an m-dimensional ($m < \infty$) set of states $\mathfrak{H}$ that is also a linear space, one might readily represent them as matrices, thus rendering E_{qt} a matrix as well. But certainly this is not the case of the harmonic oscillator, as E_{qt} has an infinity of distinct eigenvalues, and not at maximum m, as linear algebra prescribes. It seems that everything boils down to determining what is $\mathfrak{H}$, in the first place, as then we can construct fitting observables, thus connecting theory with practice.

In this subsection, we tried to illustrate the most obvious differences between classical and quantum thinking applied to a harmonic oscillator. In the remainder of this section, we will delve into how one can choose a set of states $\mathfrak{H}$ that fits the physical system under investigation, as well as sensibly define observables and solve eigenequations of the form (4) for the allowed values of physical quantities.

1.2. Setting the static quantum game: the need for Hilbert spaces and self-adjoint operators

It is a well-known fact that observables in classical mechanics take any real value, or more generally they can be anything in a **single** interval $I \subseteq \mathbb{R}$, specified by the physical context[13] [FM06]. However, a wealth of experiments attest the fact that, in certain circumstances, the observables can take only discrete values, as it was illustrated in the previous subsection for the total energy of a vibrating molecule, idealized as an harmonic oscillator. This is the case of other seemingly unconnected physical systems, such as e.g. the energy of a photon emitted via the 'lapse' of an excited electron of a hydrogen-like atom from a higher energy state to a lower energy state. Nevertheless, even in some situations where the observables take continuous values, they will lay in **multiple** intervals separated by other intervals of nonzero measure, as it was observed experimentally for the total energy of an electron in a periodic crystal lattice (according to [AdP06]).

Moreover, diffraction experiments done with photons, electrons, and even bulky molecules containing up to 2000 atoms (the experimental setup for the latter can be found in [FGZ$^+$19]) determine us to consider their *wave-like behaviour* as well when constructing a new theory to replace the often superseded CM.

The previous two observations indicate that we need a different kind of mathematics to define the observables in the quantum world. The goal of this subsection is to present the latter as clear and concise as possible.

Let us first discuss about OQM observables. Similarly to CM, where the domain

[13] For example, in the case of the harmonic oscillator, we have that the range of the total energy observable (2) is $[0, \infty) = \mathbb{R}_0^+$.

of the observables is, roughly speaking, all the momenta p and positions x allowed by the classical system under investigation, we need to specify a domain for the OQM observables as well. Having in mind the total energy observable E_{qt} for the quantum harmonic oscillator as defined in (3) and (4), we are thus led to formulate:

Axiom 1. *The states*[14] *of a quantum system are the elements ψ of a complex separable Hilbert space $\mathfrak{H}$ that satisfy $\|\psi\|_{\mathfrak{H}} = 1$.*

An OQM observable[15] *is a self-adjoint operator $A : \mathfrak{D}(A) \subseteq \mathfrak{H} \longrightarrow \mathfrak{H}$.*

For the reader unfamiliar with the terminology that we used to state Axiom 1, we kindly refer her/him to Appendix A (where we included a succinct discussion about bounded and unbounded operators as well, a topic of high relevance in this work).

Some of the technical specifications that we imposed on $\mathfrak{H}$ might be justified even at this stage: its separability is equivalent to the existence of a countable orthonormal basis [DT09, p.255], which is a useful feature if we combine it with the inherent completeness of the Hilbert space. But why do we even have a Hilbert space in the first place? Well, a Hilbert space allows us to define a self-adjoint operator A, which satisfies the 'Hermitian property' of physics $\langle A\cdot, \cdot\rangle_{\mathfrak{H}} = \langle \cdot, A\cdot\rangle_{\mathfrak{H}}$; moreover, a self-adjoint operator has real eigenvalues, a necessary condition to interpret its eigenvalues as physical quantities, as we did in (4).

It seems natural to take an OQM observable, with the domain in the *classical phase space* and try to find a corresponding one with its domain in the *quantum phase space*[16]. But how exactly are we going to do this? Obstacles seem everywhere: for example, in CM the position-momentum product is commutative (multiplication of two real numbers, $xp = px$), but nevertheless this does not hold in general for two arbitrary OQM observables A and B, i.e. $AB \neq BA$ in most of the cases. A simple example that illustrates this possible noncommutativity is when $\mathfrak{H}$ is finite-dimensional, as then linear algebra stipulates that any OQM observables A and B can be represented by a matrix (as they are in particular linear operators), and matrices may not commute. Based on

[14] To be precise, the normalized elements of $\mathfrak{H}$ correspond to the so-called *pure states*, while the full generality is obtained by considering the *mixed states* as well, which are now maps $\rho : \mathfrak{H} \longrightarrow \mathfrak{H}$. Nevertheless, it is true that for every ρ of a pure state corresponds a unique $\psi \in \mathfrak{H}$, thus allowing the identification $\psi \equiv \rho$ for a state. Although we will use mixed states latter in our development, we will write the axioms of OQM only for pure states, as the former's extra mathematical properties are not needed here (but see [Hal13, p. 419]).

[15] One might contrast this with the CM observables, which have as their codomain an interval in $\mathbb{R}$ that ensures a direct connection with empirical quantities. How do we establish the link with empirical quantities in the case of OQM? We already hinted in the previous section that by solving (4) for the eigenvalues, though the full answer awaits the reader in Axiom 3.

[16] I.e. $\mathfrak{H}$, a separable complex Hilbert space.

this observation, we introduce for latter use the map

$$[A, B] \coloneqq AB - BA, \tag{6}$$

acting on

$$\mathfrak{D}(AB) \cap \mathfrak{D}(BA) \coloneqq \{\psi \in \mathfrak{D}(B) : B\psi \in \mathfrak{D}(A)\} \cap \{\psi \in \mathfrak{D}(A) : A\psi \in \mathfrak{D}(B)\}, \tag{7}$$

and we call it the *commutator*[17].

Back to the correspondence between a CM observable satisfying certain regularity conditions and an OQM one: the procedure to obtain the latter from the former is known as the *Weyl quantization* [Hal13, p. 261]. Remember that in Subsection 1.1 we obtained E_{qt} from E_{cl} by replacing x^2 with X^2 and p^2 with P^2; at this point we are not interested in how X and P 'look', but rather in how to 'substitute' X and P in E_{cl} to obtain E_{qt}. Based on what we know from solving heuristically the quantum harmonic oscillator, we take as the quantization of E_{cl} the transformations:

$$x^2 \xrightarrow{\text{quantization}} X^2$$

and

$$p^2 \xrightarrow{\text{quantization}} P^2.$$

However, how about

$$xp \xrightarrow{\text{quantization}} XP\ ? \tag{8}$$

Could any reliable quantization scheme lead to the right-hand side of (8)? Well, in the first place, the reader might wonder why the quantization of $xp = px$ is the operator XP, and not the equally valid (from the point of view of the commutativity of the product of real numbers) PX; as we argued before, it may happen that the linear operators do not commute, hence we reached a dead end. Additionally, observe that as X and P are OQM observables, it is true that $X^* = X$ and $P^* = P$; then $(XP)^* = P^*X^* = PX$, so $XP \neq PX$ is equivalent to $XP \neq (XP)^*$ and $PX \neq (PX)^*$; without them being self-adjoint, we cannot even use them in a heuristic manner. Therefore, we should resort

[17]Clearly, as the 'products' AB and BA are nothing else than linear operators formed via the composition of two linear operators, we need to specify $\mathfrak{D}(A)$ and $\mathfrak{D}(B)$ in order for the linear operator [A,B] to exist: for example, if B is the map $\mathfrak{D}(B) \ni \psi \mapsto \|\psi\|_{\mathfrak{H}}\phi$ with $\phi \notin \mathfrak{D}(A)$, then $\nexists AB$. In view of this, (7) seems like the natural domain of $[\cdot,\cdot]$; however, there is a catch: (6) acting on (7) is the right thing only when A and B are both **bounded**, as in the case that one of them or both are unbounded, it may well happen that $\mathfrak{R}(B) \cap \mathfrak{D}(A) = \{0_{\mathfrak{H}}\}$, so AB would be defined only for the test function $\psi = 0_{\mathfrak{H}}$, thus rendering it useless (and similarly for BA). For a generalization of $[\cdot,\cdot]$ for unbounded operators, see [RS80, p.271].

to intuition: a natural proposal for the quantization of a monomial of the shape xp would then be that

$$xp \xrightarrow{\text{quantization}} \frac{1}{2}\left(XP + PX\right), \tag{9}$$

which is certainly a self-adjoint operator for X and P self-adjoint, reflects the fact that $xp = px$ as one can swap 'X' with 'P' without changing the result, and reduces to our initial guess (8) if $XP = PX$.

The generalization of (9) for monomials of the shape $x^\alpha p^\beta$, where $\alpha, \beta \in \mathbb{N}_0$, is known as the *Weyl quantization scheme*; based on (9), a reasonable candidate is

$$x^\alpha p^\beta : \xrightarrow{\text{Weyl quantization}} \frac{1}{(\alpha+\beta)!} \sum_{\sigma \in S_{\alpha+\beta}} (X \vee P)_{\sigma(1)} \dots (X \vee P)_{\sigma(\alpha+\beta)}, \tag{10}$$

with the permutation σ an element of the symmetric group[18] $S_{\alpha+\beta}$, and the self-adjoint operator

$$(X \vee P)_{\sigma(i)} \coloneqq \mathbb{1}_{\{\sigma(i) \leq \alpha\}} X + \mathbb{1}_{\{\sigma(i) > \alpha\}} P,$$

for $i \in \{1, \dots, \alpha + \beta\}$. Using (10), we can straightforwardly generalize[19] the Weyl quantization to polynomials by linearity.

We are now ready to postulate:

Axiom 2. *For every CM observable q satisfying certain conditions, the Weyl quantization scheme[20] allows us to define an OQM observable A.*

Before we can use the formalism we introduced to explicitly define the momentum and position operators, it is high time to connect the OQM observables with empirical quantities; as any apparatus provides us with real numbers that we interpret as measurements of some kind or the other, we actually have to connect the OQM observables with $\mathbb{R}$. For a self-adjoint operator A and any $\psi \in \mathfrak{H}$, we have that $\langle \psi, A\psi \rangle_{\mathfrak{H}} \in \mathbb{R}$. Let us suppose we have a particle living on the real axis, so that $\psi : \mathbb{R} \longrightarrow \mathbb{C}$. *Born's rule* of OQM [SN11, p.101] determines us to interpret $|\psi|^2$ as the probability density function (pdf) for the CM observable x, the position of the particle on the real axis. Now, we know that the complex quantity

$$\int_{\mathbb{R}} \overline{f(x)} g(x)\, dx, \tag{11}$$

[18] The set of all permutations of the elements of $\{0, \dots, \alpha + \beta\}$, which forms a group together with the operation of map composition.

[19] Although it is not very relevant for this work, the Weyl quantization can be generalized to e.g. complex exponentials as well [Hal13, p.262], an analogous development to the functional calculus we discuss in Appendix A.

[20] There are other quantization schemes [Hal13, p.258], but the Weyl quantization is the one suitable for (nonrelativistic) OQM.

for f, g elements of a convenient[21] function space $F(\mathbb{R})$, forms an inner product if we identify $\langle f, g\rangle$ with the integral above. We can then see that the expected value of the position of the particle on the real axis x, i.e.

$$E(x) \coloneqq \int_{\mathbb{R}} x|\psi(x)|^2 \, dx,$$

as prescribed by Born's rule, can be connected with $\langle \cdot, \cdot \rangle$ by rewritting

$$E(x) = \int_{\mathbb{R}} x|\psi(x)|^2 \, dx = \int_{\mathbb{R}} \overline{\psi(x)} x \psi(x) \, dx = \langle \psi, s\psi \rangle, \tag{12}$$

with s the self-map $x \mapsto x$, and assuming, of course, that ψ and $s\psi$ are elements[22] of the same function linear space as f and g, namely $F(\mathbb{R})$.

Suppose now that we have a general CM observable ą, and we wish to determine its expected value in a quantum system in a state $\psi \in F(\mathbb{R})$. It would be useful for the corresponding OQM observable A to be such that it satisfies

$$E(\text{ą}) = \langle \psi, A\psi \rangle; \tag{13}$$

in order to extend to a complex separable Hilbert space $\mathfrak{H}$ the identification of the inner product as above with the expected value, we introduce the third axiom:

Axiom 3. *If one wishes to know the expected value of a CM observable ą in a quantum system described by a state $\psi \in \mathfrak{H}$, then one should evaluate the following expression:*

$$E(\text{ą}) = \langle \psi, A\psi \rangle_{\mathfrak{H}}, \tag{14}$$

where A is the OQM observable corresponding to ą, as specified by Axiom 2.

More generally, for $m \in \mathbb{N}_0$, we have that

$$E(\text{ą}^m) = \langle \psi, A^m \psi \rangle_{\mathfrak{H}}. \tag{15}$$

If two states $\psi_1, \ \psi_2 \in \mathfrak{H}$ are connected via $\psi_1 = c\psi_2$, for a $c \in \mathbb{C}$ that satisfies[23] $|c| = 1$, then ψ_1 and ψ_2 refer to the same physical state.

The last assertion in Axiom 3 is based on the observation that

$$E(\text{ą}^m) = \langle \psi_1, A^m \psi_1 \rangle_{\mathfrak{H}} = \langle c\psi_2, A^m c\psi_2 \rangle_{\mathfrak{H}} = |c| \langle \psi_2, A^m \psi_2 \rangle_{\mathfrak{H}} = \langle \psi_2, A^m \psi_2 \rangle_{\mathfrak{H}},$$

which insinuates that even if ψ_1 and ψ_2 differ by a complex phase $c = e^{i\varphi}, \ \varphi \in \mathbb{R}$, the expected values of the empirical quantities (15) will be identical.

[21] in the sense that we can integrate the product $f\overline{g}$ of arbitrary f and g over the real axis.

[22] In '$s\psi$' we have multiplication of two functions, and not their composition!

[23] As the states should be normalized according to Axiom 1.

In light of (12) and (13), let us obtain the position operator X. Suppose that our particle[24] lives on the real axis, such that $\psi : \mathbb{R} \longrightarrow \mathbb{C}$. Recall that *Born's rule* tells us that the pdf for its position x is $|\psi|^2$. A natural candidate for the Hilbert space $\mathfrak{H}$ is then space of square-integrable functions[25] $L^2(\mathbb{R})$ endowed with the inner product (11), as then we will have that

$$\|\psi\|^2 = \langle \psi, \psi \rangle = \int_{\mathbb{R}} |\psi(x)|^2 \, dx < \infty,$$

and we know that a necessary condition for $|\psi|^2$ to be interpreted as a pdf is

$$\int_{\mathbb{R}} |\psi(x)|^2 \, dx = 1,$$

which is equivalent to $\|\psi\| = 1$. Consequently, the states are obtained by taking all $\widetilde{\psi} \in L^2(\mathbb{R})$ with $\|\widetilde{\psi}\| \neq 0$ and normalizing them, i.e. $\psi := \|\widetilde{\psi}\|^{-1}\widetilde{\psi}$. Thus, the probability that the particle is located in a Borel measurable set $\Upsilon \subseteq \mathbb{R}$ is equal to

$$\int_{\Upsilon} |\psi(x)|^2 \, dx.$$

The same as before, the expected value for the position is

$$E(x) = \int_{\mathbb{R}} x|\psi(x)|^2 \, dx, \tag{16}$$

which should be finite, as it represents the expected value of an empirical quantity; a sufficient condition for this is obviously

$$\int_{\mathbb{R}} |x||\psi(x)|^2 \, dx < \infty. \tag{17}$$

By rewriting (16) as

$$E(x) = \int_{\mathbb{R}} x|\psi(x)|^2 \, dx = \int_{\mathbb{R}} \overline{\psi(x)} x \psi(x) \, dx = \langle \psi, X\psi \rangle,$$

with $X : \mathfrak{D}(X) \subseteq L^2(\mathbb{R}) \longrightarrow M$ for an appropriate dense $\mathfrak{D}(X)$, pointwisely defined as

$$\psi(x) \longmapsto x\psi(x) \tag{18}$$

for any[26] $x \in \mathbb{R}$, we can identify[27] X via (14) as the OQM observable.

[24] In this work, the particle is assumed to be **spinless**.

[25] In fact, in order to be indeed a Hilbert space, $L^2(\mathbb{R})$ is the space of conjugacy classes of square-integrable functions that are equal almost everywhere [Rud87].

[26] Our codomain M is $\mathfrak{R}(X) := \{X\psi : \psi \in \mathfrak{D}(X)\}$, which is **not** necessarily consisting of square-integrable functions, i.e. $X\psi$ might fail to be in $L^2(\mathbb{R})$.

[27] When dealing with concrete examples, though, one must pick a suitable $\mathfrak{D}(X)$ for which $\mathfrak{R}(X) \subseteq L^2(\mathbb{R})$, as mandated by Axiom 1.

In the case of the momentum operator, things are a bit more complicated: for the position, we connected the states ψ with the expected value of empirical quantities by way of Born's rule, so we need something similar to the latter. Fortunately, the *de Broglie hypothesis* (see [Hal13, p.60]) is telling us that for a particle in the state $\psi_{\mathrm{dB}}(x,k) := e^{ikx}$, its momentum p is equal to[28] its wave's *angular wavenumber* k. However, there is a conundrum: $e^{ikx} \notin L^2(\mathbb{R})$, as one could readily verify. Our derivation fails because we insisted that our particle lives on the whole real line. In order to temporarily circumnavigate this technicality, let us consider instead as a Hilbert space the function space $L^2([0,2\pi])$ endowed with the inner product (11) adapted to $[0,2\pi]$; we specifically chose[29] $L^2([0,2\pi])$ due to the semblance of its orthonormal basis

$$\left\{ \frac{e^{ikx}}{\sqrt{2\pi}} : k \in \mathbb{Z} \right\} \tag{19}$$

to $\psi_{\mathrm{dB}}(x,k)$. Thus we can represent an element $\widetilde{\psi} \in L^2([0,2\pi])$ pointwisely as

$$\widetilde{\psi}(x) = \sum_{k=-\infty}^{\infty} \widetilde{c}_k \frac{\psi_{\mathrm{dB}}(x,k)}{\sqrt{2\pi}};$$

Parseval's identity (as in [Tes14, p.47]) implies that the norm of $L^2([0,2\pi])$ may be rewritten as

$$\|\widetilde{\psi}\|_{[0,2\pi]} = \left(\sum_{k=-\infty}^{\infty} |\widetilde{c}_k|^2 \right)^{\frac{1}{2}},$$

and the states are the normalized

$$\psi(x) = \|\widetilde{\psi}\|_{[0,2\pi]}^{-1} \widetilde{\psi}(x). \tag{20}$$

What is the momentum of the state

$$\psi(x) = \sum_{k=-\infty}^{\infty} c_k \frac{\psi_{\mathrm{dB}}(x,k)}{\sqrt{2\pi}} \ ? \tag{21}$$

The de Broglie hypothesis tells us that $\psi_{\mathrm{dB}}(x,k)$ has momentum k, so we are encouraged to interpret (21) probabilistically, i.e. the momentum will be[30] a $k \in \mathbb{Z}$ with probability $|c_k|^2$. Thus it follows that

$$E(p) = \sum_{k=-\infty}^{\infty} k|c_k|^2, \tag{22}$$

[28] We kindly remind the reader that for this part of the work we have set $\hbar = 1$; the original formula is the well-known $p = \hbar k$ ([Hal13, p.60]).

[29] In fact, any space of functions that are square-integrable over a compact interval would do the job.

[30] Notice that k is restricted to integers! It seems like we are on the good track, in light of the quantization of the energy that has been observed in experiments where the particle on a circle is an appropriate model, as is the case for the π electrons of benzene [AdP06].

a sufficient condition for interpreting (22) as representing the expected value of an empirical quantity being

$$\sum_{k=-\infty}^{\infty} |k||c_k|^2 < \infty,$$

which is analogous to (17).

We then search for an operator P that satisfies (compare with (13)):

$$E(p) = \langle \psi, P\psi \rangle_{[0,2\pi]}. \tag{23}$$

It helps to express the inner product as

$$\langle \psi, \phi \rangle_{[0,2\pi]} = \int_0^{2\pi} \overline{\psi(x)}\phi(x)\, dx = \sum_{k=-\infty}^{\infty} \overline{c_k} d_k, \tag{24}$$

for ϕ another element of $L^2([0, 2\pi])$ which was expressed with the help of the countable orthonormal basis of $L^2([0, 2\pi])$ as

$$\phi(x) = \sum_{k=-\infty}^{\infty} d_k \frac{\psi_{\mathrm{dB}}(x,k)}{\sqrt{2\pi}}.$$

Thus, (22), (23) and (24) imply that a sufficient condition that P should satisfy is

$$P\psi_{\mathrm{dB}}(x,k) = k\psi_{\mathrm{dB}}(x,k). \tag{25}$$

In turn, (25) is definitely true for

$$P : \mathfrak{D}(P) \subseteq L^2([0, 2\pi]) \longrightarrow N, \tag{26}$$

pointwisely defined as[31]

$$\psi(x) \mapsto -i\frac{d\psi(x)}{dx}, \tag{27}$$

for any $x \in [0, 2\pi]$, which we take as the momentum operator[32] for a particle on a unit circle.

[31]Technically speaking, we cannot feed in $d/\,dx$ any (normalized) $\psi \in L^2(\mathbb{R})$, as the latter might fail to be even continuous; nevertheless, the subsequent Schrödinger equation can be understood for arbitrary $\psi \in L^2(\mathbb{R})$ if we retort to the theory of *generalized distributions*, created by Laurent Schwartz, the eponym of the Schwartz space S (see Appendix D), to formalize objects like the Dirac delta function. We will not pursue this line of thought in our exposition, as by doing this little is gained from a physical point of view, but a very brief introduction can be found in [DT09, p.264-p.267].

[32]Similarly to the position operator, the domain $\mathfrak{D}(P)$ is dense, in order to have a well-defined self-adjoint operator, and also clearly $N = \{P\psi : \psi \in \mathfrak{D}(P)\}$.

Back to the particle living on the real axis. Although $\psi_{\mathrm{dB}} \notin L^2(\mathbb{R})$, owing to (25), we can use the Fourier transform to find a decomposition similar in spirit to (21), now relevant to the whole real line; for an arbitrary $\psi \in L^2(\mathbb{R})$, we then have:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} (\mathcal{F}\psi)(k) e^{ikx}\, dk = \int_{\mathbb{R}} (\mathcal{F}\psi)(k) \frac{\psi_{\mathrm{dB}}(x,k)}{\sqrt{2\pi}}\, dk, \tag{28}$$

where $\mathcal{F} : L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R})$ is the Fourier transform (see [Hal13, p.531-p.533] for a rigorous discussion about $\mathcal{F}$). By further comparing the right-hand side of (28) with (21), it seems natural to expect that $|(\mathcal{F}\psi)(k)|^2$ should play the same role as $|c_k|^2$ (encoding the pdf of k). This point of view is further strengthened by the fact that $\mathcal{F}$ is an isometry from $L^2(\mathbb{R})$ to $L^2(\mathbb{R})$ [Tes14, p.90], thus

$$\int_{\mathbb{R}} |(\mathcal{F}\psi)(k)|^2\, dk = \|\mathcal{F}\psi\|^2 = \|\psi\|^2 = 1;$$

in plain words, whenever ψ is a state, the function $|(\mathcal{F}\psi)|^2$ is automatically normalized, one of the requirements of being a pdf. Assuming that $|(\mathcal{F}\psi)|^2$ is indeed the pdf of the particle momentum k, the probability of it being in a Borel measurable $\Upsilon \subseteq \mathbb{R}$ is

$$\int_{\Upsilon} |(\mathcal{F}\psi)(k)|^2\, dk,$$

with the expected value

$$E(p) = \int_{\mathbb{R}} k|(\mathcal{F}\psi)(k)|^2\, dk. \tag{29}$$

We then look for an operator P that satisfies

$$E(p) = \langle \psi, P\psi \rangle;$$

we recognize that (29) can be rewritten as[33]

$$E(p) = \langle \mathcal{F}\psi, s\mathcal{F}\psi \rangle,$$

with $s : \mathbb{R} \longrightarrow \mathbb{R}$ the mapping $k \mapsto k$; on the other hand, the isometricity of $\mathcal{F}$ points to

$$\langle \psi, P\psi \rangle = \langle \mathcal{F}\psi, \mathcal{F}P\psi \rangle,$$

so we search for a P with the specification that

$$\langle \mathcal{F}\psi, \mathcal{F}P\psi \rangle = \langle \mathcal{F}\psi, s\mathcal{F}\psi \rangle.$$

[33]Mind the fact that in '$s\mathcal{F}\psi$' we have a multiplication between the two functions s and $\mathcal{F}\psi$, and **not** their composition.

A sufficient condition for the identity above to be true is that $\mathcal{F}P\psi = s\mathcal{F}\psi$ (recall that we chose an arbitrary $\psi \in L^2(\mathbb{R})$). This follows easily, as

$$\mathcal{F}P\psi = -i\mathcal{F}(\,d\psi/\,dk) = -i^2 s\mathcal{F}\psi = s\mathcal{F}\psi,$$

where we used a simple property that connects the Fourier transform of a function with the one of its derivative ([Tes14, p.188]). Hence, it is not presumptuous to take (26)-(27) as the momentum operator in the case of $L^2(\mathbb{R})$ as well.

In view of Axiom 2, X and P should be self-adjoint; even so, without specific $\mathfrak{D}(X)$ and $\mathfrak{D}(P)$ imposed by a concrete quantum system, we cannot show that $X = X^*$ and $P = P^*$ at this stage. Nevertheless, with a few 'common sense' assumptions, we can still infer that they are symmetric, a necessary condition for them to be self-adjoint: in the case of the position operator X, a quick manipulation shows that

$$\langle \phi, X\psi\rangle = \int_{\mathbb{R}} \overline{\phi(x)} x\psi(x)\,dx = \int_{\mathbb{R}} \overline{x\phi(x)}\psi(x)\,dx = \langle X\phi, \psi\rangle, \tag{30}$$

where we used the obvious $\overline{x} = x$, as we integrate over the real line, and we made the extra assumptions that $X\psi$, $X\phi \in L^2(\mathbb{R})$, for ψ, $\phi \in L^2(\mathbb{R})$.

Similarly, for the momentum operator P one can calculate that

$$\begin{aligned} \langle \phi, P\psi\rangle_{[-L,L]} &= \int_{-L}^{+L} \overline{\phi(x)}(-i\,d\psi(x)/\,dx)\,dx \\ &= -i\overline{\phi(x)}\psi(x)\Big|_{-L}^{+L} + \int_{-L}^{+L} \overline{(-i\,d\phi(x)/\,dx)}\psi(x)\,dx, \end{aligned} \tag{31}$$

for an arbitrary $L > 0$. As usual, in order to take $L \to \infty$ in (31) and obtain our heuristic result, one may assume that the states ψ and ϕ are vanishing[34] at the infinity of the configuration space (in our case, the real axis), i.e. $\lim_{x\to\pm\infty}\psi(x) = 0$ and $\lim_{x\to\pm\infty}\phi(x) = 0$. Therefore, as $L \to \infty$, the boundary terms become null, and for the integral on the first line of (31) we have

$$\begin{aligned} 0 &\le \left| \int_{-L}^{+L} \overline{\phi(x)}(-i\,d\psi(x)/\,dx)\,dx - \int_{-\infty}^{+\infty} \overline{\phi(x)}(-i\,d\psi(x)/\,dx)\,dx \right| \\ &\le \int_{+L}^{+\infty} \left|\overline{\phi(x)}(-i\,d\psi(x)/\,dx)\right|\,dx + \int_{-\infty}^{-L} \left|\overline{\phi(x)}(-i\,d\psi(x)/\,dx)\right|\,dx, \end{aligned}$$

which indeed shows that

$$\lim_{L\to\infty} \int_{-L}^{+L} \overline{\phi(x)}(-i\,d\psi(x)/\,dx)\,dx = \int_{-\infty}^{+\infty} \overline{\phi(x)}(-i\,d\psi(x)/\,dx)\,dx.$$

[34] A natural condition for ψ, ϕ to represent a physical state.

In order for all the integrals above to be finite when we consider them over the whole real axis, in particular $[-L, L]$, it is sufficient to take $\psi,\ \phi,\ d\psi/\,dx,\ d\phi/\,dx \in L^2(\mathbb{R})$, as then their products will be integrable[35], and $L^1(\mathbb{R}) \subsetneq L^1([-L, L])$.

The integral on the last line of (31) converges similarly to the one on the first line. We thus conclude that

$$\langle\phi, P\psi\rangle = \int_{-\infty}^{+\infty} \overline{\phi(x)}(-i\, d\psi(x)/\,dx)\, dx = \int_{-\infty}^{+\infty} \overline{(-i\, d\phi(x)/\,dx)}\psi(x)\, dx = \langle P\phi, \psi\rangle, \quad (32)$$

i.e. P is a symmetric linear operator.

We finally came with an explicit X and P to be used in (3). Thus, we have that the OQM observable for the total energy of a quantum harmonic oscillator E_{qt} is acting on a state ψ pointwisely as

$$\psi(x) \mapsto -\frac{1}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}kx^2\psi(x).$$

We mention in passing that in the general case (15), X^m and P^m look as one would expect. If we do not have information about $\mathfrak{D}(X)$ and $\mathfrak{D}(P)$ from our quantum system, one can define their nested domains[36] recursively:

$$\mathfrak{D}(X^m) = \{\psi \in \mathfrak{D}(X^{m-1}) : X\psi \in L^2(\mathbb{R})\},$$
$$\mathfrak{D}(P^m) = \{\psi \in \mathfrak{D}(P^{m-1}) : P\psi \in L^2(\mathbb{R})\},$$

where obviously $X^0 := \mathbb{I}$, $P^0 := \mathbb{I}$, such that it comes natural to define $\mathfrak{D}(X^0) := L^2(\mathbb{R})$, $\mathfrak{D}(P^0) := L^2(\mathbb{R})$; as one expects, by map composition, X^m is pointwisely the mapping

$$\psi(x) \mapsto x^m\psi(x),$$

and similarly for P^m we have

$$\psi(x) \mapsto (-i)^m\frac{d^m\psi(x)}{dx^m}.$$

To end this subsection, let us compute the commutator for X and P:

$$PX\psi(x) = -i\frac{d}{dx}(x\psi(x)) = -i\psi(x) - ix\frac{d\psi}{dx} = -i\psi(x) + XP\psi(x),$$

so

$$[X, P] = i\mathbb{I}, \quad (33)$$

for an arbitrary $\psi \in \mathfrak{D}(XP) \cap \mathfrak{D}(PX)$, and assuming that we have a nontrivial domain for the commutator $\mathfrak{D}(XP) \cap \mathfrak{D}(PX) \neq \{0_{L^2}\}$, as in (7).

[35] We use '$L^1(\Upsilon)$' to denote the linear space of integrable functions on the Lebesgue measurable set $\Upsilon \subseteq \mathbb{R}^m$, where $m \geq 1$.

[36] We generally need to propose domains for X and P on which they are self-adjoint, but here we just aim to well-define two bona fide linear operators, which, with few extra conditions, turn out to be symmetric.

1.3. Repeated measurements and the wave function collapse

Let us revisit equation (25) for a particle living on a unit circle. It says that $\psi_{\mathrm{dB}}(x,k)$ is an eigenvector of P with the eigenvalue k, where $k \in \mathbb{Z}$ is fixed. Moreover, in light of (19), we know that the eigenvectors $\{\psi_{\mathrm{dB}}(x,k)/\sqrt{2\pi} : k \in \mathbb{Z}\}$ form an orthonormal basis for $L^2\left([0,2\pi]\right)$. As we pointed before, for a general state (20), we have that the distinct eigenvalues $k \in \mathbb{Z}$ will be the result of a measurement with probability $|c_k|^2$. We are interested in obtaining theoretically the expected value for the CM observable $\utilde{a}$ of a physical system; to do this, Axiom 2 stipulates on how to choose an OQM observable A such that $\langle \psi, A\psi\rangle_{\mathfrak{H}}$ is the expected value of $\utilde{a}$. The key observation is that it is very easy to compute (15) if the state under consideration is an (linear combination of) eigenvector(s) of the OQM observable A. Formally, we can write for a state consisiting of a single eigenvector:

$$\psi \in \mathfrak{H} \text{ is a state with } A\psi = \lambda\psi \implies E(\utilde{a}) = \langle \psi, A\psi\rangle_{\mathfrak{H}} = \langle \psi, \lambda\psi\rangle_{\mathfrak{H}} = \lambda\|\psi\|^2_{\mathfrak{H}} = \lambda. \quad (34)$$

As we saw in Subsection 1.1, the total energy OQM observable E_{qt} of the harmonic oscillator has an infinity of distinct eigenvalues (5), which we collect in a set $\{\lambda_{E,n}\}_{n=1}^{\infty}$. If we solve the quantum harmonic oscillator using the 'analytic method', we obtain along the distinct eigenvalues their corresponding (linearly independent) eigenvectors $\{\psi_n\}_{n=1}^{\infty}$ (see [Hal13, p.233] for explicit formulae). Thus, it should be clear that

$$E(E_{\mathrm{cl}}) = \langle \psi, E_{\mathrm{qt}}\psi\rangle_{qho} = \lambda_{E,m},$$

if $\psi := \psi_m$, for an $m \in \mathbb{N}$, and a $\langle \cdot,\cdot\rangle_{qho}$ suitable for the quantum harmonic oscillator, as specified by the Hilbert space we use to model it.

Most generally, if[37] $\{\psi_k\}_{k\in K}$ is simultaneously an orthonormal basis and consists of eigenvectors of an OQM observable A with not necessary distinct eigenvalues $\{\lambda_j\}_{j\in J}$, and we take for convenience $J \subseteq K$, one can write an arbitrary state $\psi \in \mathfrak{H}$ as

$$\psi = \sum_{k\in K} c_k\psi_k, \quad (35)$$

which leads to the probability that a measurement will return the value $\mu \in \mathbb{R}$:

$$\zeta(\mu) := \sum_{k\in K} |c_k|^2 \mathbb{1}_{\{\psi_k \text{ s.t. } A\psi_k = \mu\psi_k\}}.$$

Consequently, the expected value of $\utilde{a}$ is given by

$$E(\utilde{a}) = \sum_{j\in J} \lambda_j \zeta(\lambda_j).$$

[37] The index set K is countable, as our Hilbert space $\mathfrak{H}$ is separable.

The previous remarks help us formulate in precise terms the following physical intuition: if we perform a measurement on a quantum system described by ψ and we find the classical observable ą to be equal to λ, and subsequently if we measure **immediately** ą once again, then the state of the quantum system when we perform the second measurement should be a $\widetilde{\psi}$ such that our apparatus will return the same value λ. This leads to:

Axiom 4. *On a quantum system in a state ψ we perform a measurement of ą that returns the value λ. Immediately after the measurement, the quantum system will be in a state $\widetilde{\psi}$ that satisfies:*

$$A\widetilde{\psi} = \lambda\widetilde{\psi}.$$

Axiom 4 ensures us that any successive measurements done very close in time one from the other will return λ, i.e. in this regime the quantum system is 'deterministic'. The passage of the state of the quantum system from ψ to $\widetilde{\psi}$ is referred to as the *wave function collapse*[38].

The wave function collapse is the controversial part of OQM, as we already pointed to in the Introduction. It motivated the creation of many of the equivalent[39] interpretations of QM, almost all of them trying to circumvent the measurement problem in one way or the other: for a recent development in this direction, the reader might be interested to glance over Gerard 't Hooft's cellular automaton interpretation of QM [tH16].

Likewise, we can point to the measurement problem[40] as the driving force behind the topic we consider in Section 3, nonrelativistic scattering of a single spinless particle that has a **position** (the latter can be done naturally using BM, often known under the name of 'de Broglie-Bohm theory'). However, for now we will accept the wave function collapse as it is: a fundamental mechanism of OQM.

In Axiom 4 we hinted at time evolution, but nevertheless we assumed that the repeated measurements are performed almost instantaneously, such that our quantum system is 'forever' locked in the state $\widetilde{\psi}$. Accordingly, inferring anything useful about the time evolution of ψ is not possible from Axiom 4; we need a connection between ψ and t, which will ultimately lead to a full description of a latter state of the quantum system $\psi(t)$. That

[38] Known in its early days under the name 'reduction of the wave packet'.

[39] In the sense of predictions of empirical quantities; with regards to the concepts underlying them, the numerous interpretations of QM to date differ wildly, see [Omn94] for a general discussion about the foundations of QM.

[40] As the reader will soon see, the strength of BM far exceeds the circumvention of the measurement problem. With its help, we can lift the veil on central aspects of mathematical scattering theory; this strengthens a belief we have about physical theories, which roughly goes along the lines: if we solve an issue that is foundational (i.e. in our case the measurement problem), many more 'applied' issues will follow suit (defining a conceptually clearer scattering cross section using BM, see Subsection 3.5 and Section 4).

is what we are going to do in the following subsection: motivate the (time-dependent) Schrödinger equation as being the link between the states a quantum system assumes at different moments of time.

1.4. Time evolution and the Schrödinger equation

As we explained in the previous subsections, the de Broglie hypothesis allows us to interpret $\psi_{\mathrm{dB}}(x,k) = e^{ikx}$ as being a state with momentum k. Similarly, the time evolution can be motivated using the following observation[41] that we owe to Max Planck (from [SN11, p.69]): the energy of the particle is connected to the angular frequency of the time-dependent state $\psi(t)$ via[42]

$$E = \omega.$$

To begin our derivation for an equation that captures the time evolution of states, suppose that H is the OQM observable obtained by quantizing

$$H_{\mathrm{cl}}(x,p) \coloneqq \frac{1}{2m}p^2 + V(x),$$

the total energy CM observable[43] of a particle subjected to a generic potential V. For a complex separable Hilbert space $\mathfrak{H}$ suitable for our physical system, we first try to derive an equation for the normalized eigenfunctions of H; the definition of a normalized eigenfunction $\psi \in \mathfrak{H}$ is that

$$H\psi = E\psi, \tag{36}$$

with $\|\psi\|_{\mathfrak{H}} = 1$, so our quantum system has the definite energy E, which is of course a real number (as H is an OQM observable). But how may we 'combine' ω and t with ψ, in order to obtain $\psi(t)$? Ideally, if $\psi \in \mathfrak{H}$, then we should have[44] that $\psi(t) \in \mathfrak{H}$ as well; additionally, it comes natural to require that $\|\psi(t)\|_{\mathfrak{H}} = 1$, so that states evolve into other states. The simplest way to meet both requirements is by way of taking

$$\psi(t) = c(t,\omega)\psi, \text{ with } |c(t,\omega)| = 1. \tag{37}$$

[41] Although Planck postulated his 'energy quanta' in order to circumvent the ultraviolet catastrophe that plagued the continuous-energy model for the spectral radiance of a black body proposed by Lord Rayleigh and Sir James Jeans, he assigned the success of this rather odd solution to a yet to be elucidated mechanism that manifests in the walls of the black-lined cavity, and not as a fundamental property of the electromagnetic radiation **inside the cavity**; it was Einstein who set forth the latter viewpoint, a great paradigm shift from the predictions of CM [Kuh96].

[42] In original $E = \hbar\omega$, as it appears also in [SN11, p.69].

[43] The details of quantizing V can be found in Subsection 1.5; E_{qt} as in (3) is the quantization for the particular case of elastic potential $V(x) \coloneqq (k/2)x^2$.

[44] E.g. the particle on the real axis has associated a square-integrable function $\psi \in L^2(\mathbb{R})$ that we use to model various physical phenomena, owing to the nice properties of $L^2(\mathbb{R})$; it would be impractical, not to mention slightly unphysical, if in our theory $\psi(t)$ is not square-integrable anymore.

Now, observe that

$$e^{-i\omega t}\psi_{\mathrm{dB}}(x,k) = e^{i(kx-\omega t)}$$

is the prototypical unit plane wave with phase speed $v \coloneqq \omega/k$. Thus, choosing

$$\psi(t) = e^{-iEt}\psi, \text{ with } c(t,\omega) = e^{-i\omega t} = e^{-iEt}$$

as the time evolution of a state ψ with definite energy E seems legitimate[45], in view of (37). The eigenfunction ψ is called a *stationary state*, reflecting the fact that it is equivalent to its time evolved state $\psi(t)$ (see Axiom 3 and the comments below). We will then refer to (36) as the *time-independent Schrödinger equation.* However, as we are interested in time evolution, it is instructive to differentiate the equation above:

$$\frac{d}{dt}\psi(t) = -iEe^{-iEt}\psi = -iE\psi(t) = -iH\psi(t), \tag{38}$$

where we used (36) in the last step. The straightforward generalization of (38) to a state that is not necessary an eigenvector of H sets forth the following axiom:

Axiom 5. *The time evolution of a state $\psi(t) \in \mathfrak{D}(H)$ is given by*

$$\frac{d}{dt}\psi(t) = -iH\psi(t), \tag{39}$$

where H is the OQM observable corresponding to the total energy CM observable H_{cl}, as prescribed by Axiom 2.

We call (39) the *time-dependent Schrödinger equation.* With it and the previous axioms, we have the main ingredients that a good physical theory should entail. As a safety check, we can easily show that $\psi(t)$ stays normalized even if the initial state ψ (i.e. $\psi(0) \coloneqq \psi$) is not necessary an eigenvector of H, but a general solution of (39), i.e.

$$\begin{aligned}
\frac{d}{dt}\|\psi(t)\|^2_{\mathfrak{H}} &= \frac{d}{dt}\langle\psi(t),\psi(t)\rangle_{\mathfrak{H}} \\
&= \left\langle \frac{d}{dt}\psi(t),\psi(t)\right\rangle_{\mathfrak{H}} + \left\langle \psi(t),\frac{d}{dt}\psi(t)\right\rangle_{\mathfrak{H}} \\
&= \langle -iH\psi(t),\psi(t)\rangle_{\mathfrak{H}} + \langle\psi(t),-iH\psi(t)\rangle_{\mathfrak{H}} \\
&= -\langle iH\psi(t),\psi(t)\rangle_{\mathfrak{H}} + \langle iH\psi(t),\psi(t)\rangle_{\mathfrak{H}} \\
&= 0,
\end{aligned} \tag{40}$$

where we markedly used the fact that $H = H^*$. Nevertheless, in order to justify with rigour (40), further mathematics has to be introduced—as our immediate scope after

[45] If we assume that $\hbar = 1$, like we did in this subsection, then the unit of E is s^{-1}, so Et is dimensionless, thus a suitable choice for an exponent.

introducing Axiom 5 is to justify it from a physical point of view, we drop the rigour from now on, relegating to Appendix A all the mathematical details that we skip.

We thus turn our attention to the time evolution of the expected values of empirical quantities, namely how does the time-dependent version of (14), i.e.

$$\langle A\rangle_{\psi(t)} \coloneqq \langle \psi(t), A\psi(t)\rangle_{\mathfrak{H}}, \tag{41}$$

change with time? There is only one way we can answer this question, by calculating

$$\begin{aligned}
\frac{d}{dt}\langle A\rangle_{\psi(t)} &= \left\langle \frac{d}{dt}\psi(t), A\psi(t)\right\rangle_{\mathfrak{H}} + \left\langle \psi(t), A\frac{d}{dt}\psi(t)\right\rangle_{\mathfrak{H}} \\
&= i\,\langle H\psi(t), A\psi(t)\rangle_{\mathfrak{H}} - i\,\langle \psi(t), AH\psi(t)\rangle_{\mathfrak{H}} \\
&= i\,\langle \psi(t), HA\psi(t)\rangle_{\mathfrak{H}} - i\,\langle \psi(t), AH\psi(t)\rangle_{\mathfrak{H}} \\
&= -i\,\langle \psi(t), [A,H]\psi(t)\rangle_{\mathfrak{H}} \\
&= -i\,\langle [A,H]\rangle_{\psi(t)}\,,
\end{aligned}$$

which is important enough to recast it in its final form:

$$\frac{d}{dt}\langle A\rangle_{\psi(t)} = -i\,\langle [A,H]\rangle_{\psi(t)}\,. \tag{42}$$

Equation (42) tells us that noncommutativity of OQM observables H and A is an essential ingredient of OQM; without it, we would have that $\langle A\rangle_{\psi(t)} =$ constant, i.e. a conserved quantity. However, it is **not** reasonable to expect that any significant OQM observable A does not commute with H: similarly to CM, conserved quantities are expected to exist and provide us with insights regarding the physical system under analysis (for example, we do have that for a particle under the influence of a central potential V, the OQM observables corresponding to the x, y, z components of the orbital angular momentum CM observable do commute with the Hamiltonian, as one would expect [SN11, p.207]).

Speaking of CM, one might have noticed the semblance between

$$\frac{d}{dt}\langle X\rangle_{\psi(t)} = -i\,\langle [X,H]\rangle_{\psi(t)}\,, \quad \frac{d}{dt}\langle P\rangle_{\psi(t)} = -i\,\langle [P,H]\rangle_{\psi(t)}$$

and Hamilton's equations introduced at the beginning of Subsection 1.1:

$$\frac{d}{dt}x(t) = \{x(t), H_{\mathrm{cl}}(t)\}, \quad \frac{d}{dt}p(t) = \{p(t), H_{\mathrm{cl}}(t)\}, \tag{43}$$

where, contrary to (1), we stressed the time dependence. This further insinuates that the map

$$(A,B) \mapsto -i[A,B]$$

is the OQM counterpart of the CM map

$$(a,b) \mapsto \{a,b\},$$

where A, B are two OQM observables obtained through Axiom 2 from the CM observables a and b; even the properties of $[\cdot,\cdot]$ mimic the ones of $\{\cdot,\cdot\}$, as one can readily see from comparing [Hal13, p.73] with [FM06, p.378].

The remarks above inspire us to further study the connections between OQM and CM: as (41) represents the expected value of an empirical quantity, we reckon that it will manifest classical features in certain contexts. We will investigate this hypothesis in the next subsection.

1.5. Recovering classical mechanics from orthodox quantum mechanics, at least on average

Let us get back to the particle living on the real axis, for which $\mathfrak{H} := L^2(\mathbb{R})$. In order to compute (42) for X and P, we need to quantize

$$H_{\mathrm{cl}}(x,p) = \frac{1}{2m}p^2 + V(x). \tag{44}$$

Weyl's quantization scheme straightforwardly implies that the quantization of p^2 is P^2 as in (27). For $V(x)$, however, the matter is a little bit more complicated: heuristically, we can imagine the ensuing OQM observable as being obtained by 'composing' V with the position operator X defined in (18), such that we obtain another operator 'V(X)' pointwisely defined as

$$\psi(x) \longmapsto V(x)\psi(x),$$

i.e. multiplication of the evaluation of the state ψ at x with the scalar $V(x)$. Nevertheless, although this seems like the natural approach in this case, it is not rigorous, and even further from being general, as, for example, if we have

$$\underset{\sim}{a}(x,p) = e^p,$$

then what is really the mathematical meaning of

$$\text{“}A = e^P = e^{-i\frac{d}{dx}}\text{”},$$

obtained in the same way as $V(X)$? With this in mind we created the last part of Appendix A, where we discuss the far-ranging implications of having a 'functional calculus', i.e. of making sense of expressions of the type '$f(A)$', where A is a self-adjoint operator and f a real-valued function obeying certain conditions.

Back to the particle on the real axis. We just argued that the quantization of H_{cl} is

$$H = -\frac{1}{2m}\frac{d^2}{dx^2} + V(X),$$

acting on the state ψ at a point in space $x \in \mathbb{R}$

$$\psi(x) \mapsto -\frac{1}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x).$$

We are then ready to calculate the commutator of H with X and P, as we are interested in what (42) has to tell us about the 'dynamics' of $\langle X\rangle_{\psi(t)}$ and $\langle P\rangle_{\psi(t)}$. We will present in detail the simplest computation, i.e.

$$\begin{aligned}
[X,H]\psi(x) &= (XH - HX)\psi(x) \\
&= xH\psi(x) - Hx\psi(x) \\
&= -\frac{x}{2m}\frac{d^2}{dx^2}\psi(x) + xV(x)\psi(x) \\
&+ \frac{x}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{2}{2m}\frac{d}{dx}\psi(x) \\
&- V(x)x\psi(x,t) \\
&= \frac{1}{m}\frac{d}{dx}\psi(x) \\
&= \frac{i}{m}P\psi(x),
\end{aligned}$$

so that by (42) we have

$$\frac{d}{dt}\langle X\rangle_{\psi(t)} = \frac{1}{m}\langle P\rangle_{\psi(t)}, \tag{45}$$

which is strongly reminding us of the prominent CM equation

$$\frac{d}{dt}x(t) = \frac{1}{m}p(t).$$

Similar computations lead us to

$$[P,H]\psi(x) = -iV'(X)\psi(x),$$

where $V'(X)$ is the operator that maps pointwisely $\psi(x) \mapsto V'(x)\psi(x)$; one can then substitute $[P,H]$ in (42) to obtain

$$\frac{d}{dt}\langle P\rangle_{\psi(t)} = -\langle V'(X)\rangle_{\psi(t)}, \tag{46}$$

which is reminescent of

$$\frac{d}{dt}p(t) = -V'(x(t)),$$

for a potential V connected with a central force $F(t) = -V'(x(t))$, as specified by Newton's second law.

However, we can[46] do better: turning once again our attention to H_{cl} as in (44), Hamilton's equations for position and momentum are

$$\begin{aligned}\frac{d}{dt}x(t) &= \{x(t), H_{\text{cl}}(x(t), p(t))\} \\ &= \left(\frac{\partial x}{\partial x}\frac{\partial H_{\text{cl}}}{\partial p} - \frac{\partial H_{\text{cl}}}{\partial x}\frac{\partial x}{\partial p}\right)(t) \\ &= \left(\frac{\partial H_{\text{cl}}}{\partial p}\right)(t) \\ &= \frac{1}{m}p(t)\end{aligned} \tag{47}$$

and

$$\begin{aligned}\frac{d}{dt}p(t) &= \{p(t), H_{\text{cl}}(x(t), p(t))\} \\ &= \left(\frac{\partial p}{\partial x}\frac{\partial H_{\text{cl}}}{\partial p} - \frac{\partial H_{\text{cl}}}{\partial x}\frac{\partial p}{\partial p}\right)(t) \\ &= \left(-\frac{\partial H_{\text{cl}}}{\partial x}\right)(t) \\ &= -V'(x(t)).\end{aligned} \tag{48}$$

The equations (45) and (46) are collectively known by the name of *Ehrenfest's theorem*. By comparing (47) with (45), we see that the average of the simultaneous measurements of positions performed on many quantum systems all prepared in the state $\psi(t)$ behaves in accordance to the laws of CM, plain and simple; if one looks closely at equation (46), though, we see that it needs to be true that

$$\langle V'(X)\rangle_{\psi(t)} = V'(\langle X\rangle_{\psi(t)}) \tag{49}$$

so that we can establish a clear connection with CM. Subsequently, it is not hard to find some simple situations in which (49) fails to hold (in [Hal13, p.77-p.78]); on the other hand, a sufficient informal condition for it to be true can be obtained by turning to $V(x)$ and its Taylor series around the point $x = \langle X\rangle_{\psi(t)}$:

$$\begin{aligned}V'(x) = V'(\langle X\rangle_{\psi(t)}) &+ \left[x - \langle X\rangle_{\psi(t)}\right] V''(\langle X\rangle_{\psi(t)}) \\ &+ \frac{1}{2}\left[x - \langle X\rangle_{\psi(t)}\right]^2 V'''(\langle X\rangle_{\psi(t)}) + O\left(\left[x - \langle X\rangle_{\psi(t)}\right]^3\right),\end{aligned} \tag{50}$$

where we assumed the standard conditions on $V'(x)$ such that its Taylor series can be effectively used for approximations in a neighbourhood of $x = \langle X\rangle_{\psi(t)}$. We approximate

[46] Better, but nevertheless not really surprising, as the Hamiltonian and Newtonian mechanics are both formulations of the same thing, i.e. CM.

$V'(x)$ by truncating the expansion (50) after the second-order term, we quantize the result, and then finally take the expected value (41) of the approximation to obtain

$$\langle V'(X)\rangle_{\psi(t)} \approx V'(\langle X\rangle_{\psi(t)}) + \frac{1}{2}\left\langle \left[X - \langle X\rangle_{\psi(t)}\mathbb{I}\right]^2 \right\rangle_{\psi(t)} V'''(\langle X\rangle_{\psi(t)}),$$

such that one can immediately see that if the variance of the position is negligible, i.e.

$$\left\langle \left[X - \langle X\rangle_{\psi(t)}\mathbb{I}\right]^2 \right\rangle_{\psi(t)} \tag{51}$$

is small, then naturally (49) can be taken to be true. This is just what is expected from a physical point of view, as a state $\psi(t)$ for which (51) is small indicates that the position of the particle is well-localized, which is a feature pertaining to CM.

If one is worried that (49) is an esoteric mathematical condition that has little to do with physically significant $V(x)$, then a straightforward[47] computation for the quadratic potential $V(x) = cx^2$, where $c \in \mathbb{R}$ is a constant[48], leads to

$$V'(x) = 2cx \xrightarrow{\text{Weyl quantization}} V'(X) = 2cX,$$

so that

$$\langle V'(X)\rangle_{\psi(t)} = 2c\langle X\rangle_{\psi(t)} = V'(\langle X\rangle_{\psi(t)}).$$

To conclude, in this subsection we showed that for a particle living on the real axis and for which (49) is met, in view of (47) and (48), the expected values $\langle X\rangle_{\psi(t)}$ and $\langle P\rangle_{\psi(t)}$ solve Hamilton's equations (43); one might say that we 'reconciled' OQM with CM, but nevertheless this affirmation should be taken with a grain of salt: in the next subsection, we will introduce *Heisenberg's uncertainty principle*, which is a bold breakaway from the predictions of CM.

1.6. Heisenberg's uncertainty principle

As we pointed out in the case of (42), we need to have noncommutativity of an OQM observable A with H in order to observe that the expected value of A changes with time. Similarly, Heisenberg's uncertainty principle is another consequence of noncommutativity, now between X and P, as can be seen in (33). Formally, we have:

[47]Note that in this simple case the potential is a monomial, so we can directly apply Weyl's quantization scheme (10) to it.

[48]E.g. if we take $c = (1/2)k$, for $k > 0$ the spring constant, then we obtain the elastic potential, familiar from Subsection 1.1, where it gives rise to a harmonic oscillator.

Theorem 1.1 (Generalized Heisenberg's uncertainty principle)**.** *For two symmetric operators A and B that render $\mathfrak{D}(AB)\cap\mathfrak{D}(BA) \neq \{0_{\mathfrak{H}}\}$, and a state $\psi \in \mathfrak{D}(AB)\cap\mathfrak{D}(BA)$, it holds true that*

$$\Delta_\psi(A)\Delta_\psi(B) \geq \frac{1}{2}\sqrt{|\langle [A,B]\rangle_\psi|}, \tag{52}$$

where

$$\Delta_\psi(A) \coloneqq \sqrt{\langle [A-\langle A\rangle_\psi \mathbb{I}]\,\psi, [A-\langle A\rangle_\psi \mathbb{I}]\,\psi\rangle_{\mathfrak{H}}}, \tag{53}$$

and $\Delta_\psi(B)$ is obtained by replacing 'A' with 'B' in (53).

For brevity, we will not provide a proof for Theorem 1.1 in here, but we warmly refer the reader to [Tes14, p.241-p.243] for a comprehensive discussion.

Now, notice that by using the fact that $A-\langle A\rangle_\psi\mathbb{I}$ symmetric if and only if A symmetric (follows from $\langle A\rangle_\psi \in \mathbb{R}$), the square of (53) can be rewritten as

$$\Delta^2_\psi(A) \coloneqq \left\langle \psi, [A-\langle A\rangle_\psi \mathbb{I}]^2\,\psi\right\rangle_{\mathfrak{H}}, \tag{54}$$

with the further assumption that $\psi \in \mathfrak{D}(AB)\cap\mathfrak{D}(BA)\cap\mathfrak{D}(A^2)$. We then have that (54) is the variance in the measurements of the CM variable $\mathfrak{a}$, as we already noted for (51).

Back to the particle on the real line. A surprising feature of Heisenberg's uncertainty principle is that one does not expect it from a priori pure reasoning about the nature; instead, it arises directly from a fortunate cancellation in the right-hand side of (52). We showed in (30) and (32) that X and P are symmetric[49] for certain plausible assumptions. Therefore, by using (33), (52) turns into

$$\Delta_\psi(X)\Delta_\psi(P) \geq \frac{1}{2}, \tag{55}$$

which is the celebrated inequality of Heisenberg's uncertainty principle. Conceptually it says that one cannot measure **simultaneously** the position and momentum with arbitrary precision: if one knows at an instant of time quite well where a particle is, then its momentum will be at the same instant a poorly known quantity, owing to the $1/2$ on the right-hand side of (55), and vice versa; more precisely, if $\operatorname{supp}|\psi|^2 \coloneqq \{x\in\mathbb{R} : |\psi(x)|^2 \neq 0\}$ is e.g. a small interval, then $\operatorname{supp}|\mathcal{F}\psi|^2 \coloneqq \{k\in\mathbb{R} : |\mathcal{F}\psi(k)|^2 \neq 0\}$ cannot be a small interval as well: $|\mathcal{F}\psi(k)|^2$ will be 'spread' all over the place!

We point that Theorem 1.1 seems a little bit rigid, in the sense that it is applicable for rather specific states $\psi \in \mathfrak{D}(AB)\cap\mathfrak{D}(BA)$. We cannot do much about it, as this is the price for using the commutator. Nevertheless, as by construction $\mathfrak{D}(AB)\cap\mathfrak{D}(BA) \subseteq \mathfrak{D}(A)\cap\mathfrak{D}(B)$, one might wonder whether the equivalent of (55) for A and B does not hold for the latter more physically realistic domain as well, which is larger than the

[49] See [Hal13, Ch.9.8] for the natural domains of self-adjointness, which are also the ones of symmetricity.

natural domain of $[\cdot,\cdot]$. Unfortunately, the latter hypothesis is false for general symmetric A and B. A counterexample that is very instructive can be built even with X and P: set $\mathfrak{H} \coloneqq L^2([-1,1])$, for which we will have that X is self-adjoint, in particular symmetric, on all $L^2([-1,1])$, so we can take $\mathfrak{D}(X) = L^2([-1,1])$, and further assume that[50] $\mathfrak{D}(P) = \{\psi \in C^1([-1,1]) : \psi(-1) = \psi(1)\}$, which also implies that P is symmetric. Thus, one can show [Hal13, p.245-246] that there exist states $\psi \in \mathfrak{D}(X) \cap \mathfrak{D}(P)$ for which $\Delta_\psi(P) = 0$.

Fortunately, in the case $\mathfrak{H} = L^2(\mathbb{R})$, (55) holds for all $\psi \in \mathfrak{D}(X) \cap \mathfrak{D}(P)$ [Hal13, p.246], which is certainly a better situation, an extension of the natural domain of $[\cdot,\cdot]$. It is then intuitive to wonder whether the inequality in (55) is sharp; to put it another way, does there exist (at least) a $\psi \in \mathfrak{D}(X) \cap \mathfrak{D}(P)$ that satisfies

$$\Delta_\psi(X)\Delta_\psi(P) = \frac{1}{2} \ ?$$

The answer is yes [Tes14, p.209], if and only if the state is in the set

$$\{\psi \in \mathfrak{D}(X) \cap \mathfrak{D}(P) : \exists \eta \in \mathbb{R}_{\neq 0},\ \lambda \in \mathbb{C} \text{ with } (X + i\eta P)\psi = \lambda\psi\}, \tag{56}$$

which can be made explicit by solving the ODE on the right-hand side:

$$\begin{aligned} \psi(x) &= c \exp\left\{ -\frac{(x - \langle X\rangle_\psi)^2}{2\eta} + i\langle P\rangle_\psi x \right\} \\ &= c\sqrt{2\pi\eta}\exp\{i\langle P\rangle_\psi x\}\,\mathcal{N}\left(\langle X\rangle_\psi, \sqrt{\eta}\right), \end{aligned} \tag{57}$$

with $\mathcal{N}(\cdot,\cdot)$ denoting the Gaussian distribution, and

$$\begin{aligned} \langle X\rangle_\psi &= \operatorname{Re}(\lambda) \\ \langle P\rangle_\psi &= \frac{1}{\eta}\operatorname{Re}(\lambda), \end{aligned}$$

where obviously the arbitrary $c \in \mathbb{C}$ is such that $\|\psi\| = 1$, as the states are the normalized elements of $L^2(\mathbb{R})$ by Axiom 1, and we further assumed that $\eta > 0$ (for $\eta < 0$, (56) is the empty set, as though $\psi = 0_{L^2}$ satisfies the defining ODE even in this case, it can never represent a state of a given quantum system, as it is not normalizable).

The Gaussian wave packets (57) are known by the name of *minimum uncertainty states*. They provide insights into how much the precision can be 'stretched' when one measures position and momentum in a quantum system with state ψ.

[50] With '$C^1([-1,1])$' we refer to the linear space of continuosly differentiable complex-valued functions defined on $[-1,1]$.

1.7. Nature is nonlocal, and orthodox quantum mechanics follows suit

When OQM was in its infancy, many scientists were unsettled with its apparently lax way of dealing with one of the cornerstones of modern physics: *the principle of locality*, i.e. the unreasonableness[51] of *non-informational superluminal action between spacelike separated events* (NISA).

But first things first: it was held by many that OQM is *incomplete*, i.e. that (39) is not the whole story when one talks about the time evolution of a quantum system; by adding another quantity besides the wave function ψ to model the physical reality, they hoped to fix the measurement problem. The link with nonlocality came from no one else but Albert Einstein himself, who together with Boris Podolsky and Nathan Rosen introduced in 1935 a thought experiment [EPR35] which is now known as the *EPR paradox*. By assuming that the principle of locality should be incorporated in every theory of Nature, the thought experiment lead them to conclude:

'While we have thus shown that the wave function does not provide a complete description of the physical reality, we left open the question of whether or not such a description exists. We believe, however, that such a theory is possible.'

The reply to this came the same year from one of the fiercest supporters of the completeness of the OQM, the famed Niels Bohr, who argued [Boh35] that the way the measurement is considered in [EPR35] is fallacious; hence, the matters reached a nervous stalemate for a couple of years. Later on, in 1951, David Bohm came up with a similar thought experiment, this time involving a realistic experimental setup, that reinforced the EPR paradox, while successfully circumventing Bohr's objections to the original work of Einstein et al.; the mystery deepened, the physicists were more than ever split into two camps. However, in 1964, John Stewart Bell rocked the boat with his groundbreaking paper [Bel64], where he argued that OQM should be inherently *nonlocal*, in the sense that NISA is a perfectly reasonable and necessary feature of OQM. Experimental confirmation of Bell's work came in 1972 [FC72], but nevertheless the physics community was fast at pointing out certain 'loopholes', i.e. detector errors or doubts regarding the correct experimental implementation of the OQM measurement, that may deem the pioneering work of Stuart J. Freedman and John Clauser[52] irrelevant.

[51] Although causality in special relativity explicitly forbids *informational superluminal action between spacelike separated events* (ISA), viz. a signal that is sent with a speed greater than the one of light between spacelike separated events, many physicists at that time, most notoriously Albert Einstein, wholeheartedly believed that any type of nonlocal action, be it informational or non-informational, is unphysical.

[52] Interestingly enough, Stuart J. Freedman carried his famous experiment as part of his PhD thesis,

Nevertheless, in the subsequent years, various teams of experimentalists used increasingly creative experimental setups to circumvent part of the loopholes the previous experiments were accused to suffer from: most notably in 1982, Alain Aspect et al. [ADR82] drew inspiration from Bell's subsequent work on the issue to devise a *Bell test* that was met with widespread acceptance[53] by the scientific community.

In this subsection, we will first consider Bohm's variant of EPR paradox (EPRB), as Bell did in his original paper. This paves the way to Bell's theorem, which proves that OQM is compatible with EPRB only if we assume that OQM embodies NISA.

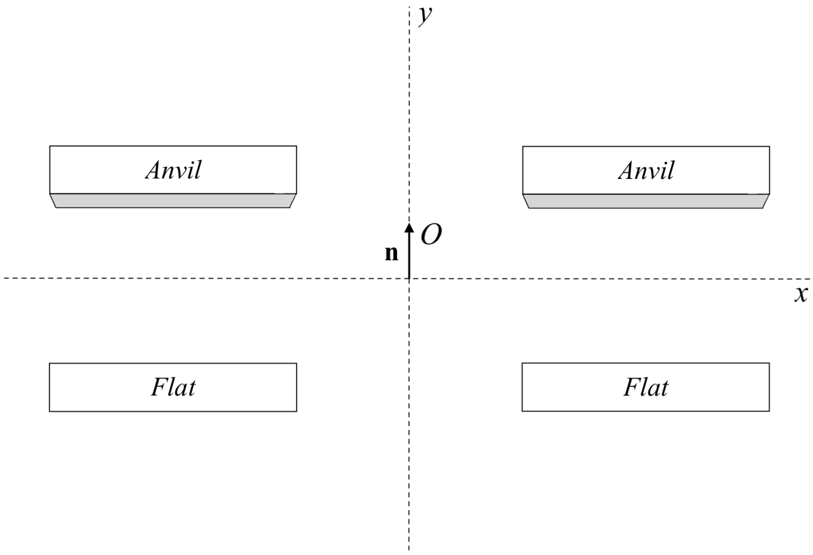

Figure 1: Two Stern-Gerlach magnets with the orientation **n**.

In Figure 1 we sketched the basic components of EPRB: two Stern-Gerlach magnets[54] oriented in the **n** direction and situated on the left (SG-L) and right (SG-R), respectively, and separated by a considerable distance, such that we can be sure that the measurements at SG-L and SG-R will always be spacelike separated events; in the middle, at O, two

having John Clauser as his advisor.

[53] Alas, every Bell test has loopholes by the very nature of experimentation, so devising new ones is an active field of research.

[54] The purpose of the asymmetric configuration of an anvil-shaped magnet and a flat one is to create an inhomogeneous magnetic field that will modify the direction of a perpendicular beam of electrons in upward and downward parts, respectively, thus forcing to theorize the existence of an inherently quantum mechanical discretized quantity, i.e. spin. As it happens, the original experiment conceived by Otto Stern and conducted by Walther Gerlach was similar in spirit, but it used instead a beam of silver atoms to show that the orbital angular momentum is quantized [GS22]. For an excellent review of the Stern-Gerlach experiment, the reader might wish to consult [SN11].

electrons prepared in a state[55]

$$\Psi(\mathbf{x_1}, \mathbf{x_1}) \otimes \Psi_{\text{singlet}},$$

where

$$\Psi(\mathbf{x_1}, \mathbf{x_1}) = \Psi_{\mathrm{L}}(\mathbf{x_1})\Psi_{\mathrm{R}}(\mathbf{x_2}) + \Psi_{\mathrm{R}}(\mathbf{x_1})\Psi_{\mathrm{L}}(\mathbf{x_2})$$

is the symmetric position-dependent wave function that corresponds to one electron moving to the left and the other to the right, and [56]

$$\Psi_{\text{singlet}} = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2\right) \tag{58}$$

is the asymmetric singlet wave function, as prescribed by the *Pauli exclusion principle*, with[57] $\langle \uparrow | \downarrow \rangle_i \coloneqq |\uparrow\rangle_i |\downarrow\rangle_i = 0,\ i = 1, 2$.

If, say, the electron that passes through the inhomogeneous magnetic field of SG-L is deflected upwards, viz. it has $\mathbf{n}$-spin $+1/2$, then the other will be diverted downwards once it passed through SG-R, which means that it has $\mathbf{n}$-spin $-1/2$, and vice versa; the probability for one of these mutually exclusive events (L-up and R-down, versus L-down and R-up) is equal to 1/2, as it can be inferred directly from the singlet state (58).

We then assume that ISA does not manifest, i.e. by the fact that SG-R and SG-L are spacelike separated, a light signal cannot communicate the measurement of the $\mathbf{n}$-spin of the R-electron at SG-R to the L-electron before the latter passes through SG-L, and the other way around. An immediate consequence of not ISA is that the values of $\mathbf{n}$-spin measured at SG-L and SG-R are preexisting, namely if e.g. we measure L-up, this would not influence the outcome[58] we get at SG-R. Along the same lines, suppose the electrons start to fly to the right and left, respectively, and before they reach SG-R and SG-L, we pick the orientations of the latter as $\mathbf{n}$. Consequently, if the values preexist, then they preexist even before we decided on a particular $\mathbf{n}$. In view of this, it comes handy to collect these measurements using the following random variables

$$X_{\mathbf{n}}^{L,R} \in \left\{+\frac{1}{2}, -\frac{1}{2}\right\},$$

where it holds true by the preceding discussion that the values are *anti-correlated*:

$$X_{\mathbf{n}}^{R} = -X_{\mathbf{n}}^{L}, \tag{59}$$

[55] The symbol '$\otimes$' is the tensor product we use to consider both Ψ and Ψ_{singlet} at the same time; for a rigorous definition, see [DT09, p.271-p.276].

[56] Nonetheless, to keep our presentation succint, we will not introduce OQM's take on spin in here, but refer the reader to [SN11]).

[57] We will occasionally resort to Dirac notation for conciseness.

[58] There is a great difference between the banal 'learning at a distance' and the spectacular nonlocality that EPRB refers to, as Bell himself indicated in the whimsical article [Bel81].

so

$$P\left(\left\{X_{\mathbf{n}}^{R}=-X_{\mathbf{n}}^{L}\right\}\right)=1 \text{ and } P\left(\left\{X_{\mathbf{n}}^{R}=X_{\mathbf{n}}^{L}\right\}\right)=0.$$

Suppose we wish to measure the spin in three arbitrary orientations, $\mathbf{n}_1$, $\mathbf{n}_2$ and $\mathbf{n}_3$. We will ask a rather odd question, atoning for it a later stage: what can we say about the sum of the probabilities of $X_{\mathbf{n}_1}^{R}$, $X_{\mathbf{n}_2}^{R}$ and $X_{\mathbf{n}_3}^{R}$, respectively, being non-trivially **anti-correlated** between them?

The sum in question is

$$\sum_{1\leq i<j\leq 3} P\left(\left\{X_{\mathbf{n}_i}^{R}=-X_{\mathbf{n}_j}^{L}\right\}\right). \tag{60}$$

Well, certainly we can use (59) to infer that the sum above is the same as

$$\sum_{1\leq i<j\leq 3} P\left(\left\{X_{\mathbf{n}_i}^{R}=X_{\mathbf{n}_j}^{R}\right\}\right), \tag{61}$$

which can be lower-bounded by rearranging the well-known inclusion-exclusion principle

$$P\left(\bigcup_{i=1}^{3} A_i\right)=\sum_{i=1}^{3} P\left(A_i\right)-\sum_{1\leq i<j\leq 3} P\left(A_i\cap A_j\right)+P\left(\bigcap_{i=1}^{3} A_i\right)$$

into

$$\begin{aligned}\sum_{i=1}^{3} P\left(A_i\right) &= P\left(\bigcup_{i=1}^{3} A_i\right)-P\left(\bigcap_{i=1}^{3} A_i\right)+\sum_{1\leq i<j\leq 3} P\left(A_i\cap A_j\right)\\ &\geq P\left(\bigcup_{i=1}^{3} A_i\right),\end{aligned} \tag{62}$$

as e.g. $A_1 \cap A_2 \supseteq \bigcap_{i=1}^{3} A_i$, thus rendering positive the difference between the last two terms in the first line of the inequality above.

Thereafter, take the events

$$A_1 \coloneqq \left\{X_{\mathbf{n}_1}^{R}=X_{\mathbf{n}_2}^{R}\right\}, \quad A_2 \coloneqq \left\{X_{\mathbf{n}_1}^{R}=X_{\mathbf{n}_3}^{R}\right\}, \quad A_3 \coloneqq \left\{X_{\mathbf{n}_2}^{R}=X_{\mathbf{n}_3}^{R}\right\}, \tag{63}$$

where the reader should beware the slightly confusing indices in (63), as well as the fact that the cross-sum term $\sum_{1\leq i<j\leq 3}$ in (62) does **not** correspond to the cross-sum one in (61). Thus, we can lower-bound the aforementioned sum as

$$\sum_{1\leq i<j\leq 3} P\left(\left\{X_{\mathbf{n}_i}^{R}=X_{\mathbf{n}_j}^{R}\right\}\right)\geq P\left(\bigcup_{1\leq i<j\leq 3}\left\{X_{\mathbf{n}_i}^{R}=X_{\mathbf{n}_j}^{R}\right\}\right), \tag{64}$$

and we observe that the event measured on the right-hand side of (64) is a sure one, as we have three random variables $X_{\mathbf{n}_1}^{R}$, $X_{\mathbf{n}_2}^{R}$ and $X_{\mathbf{n}_3}^{R}$, and **only** two values they can assume, i.e. $\{+1/2, -1/2\}$. Hence, we arrive at (one of the variants of) *Bell's inequality*, namely

$$\sum_{1\leq i<j\leq 3} P\left(\left\{X^R_{\mathbf{n}_i} = X^R_{\mathbf{n}_j}\right\}\right) \geq 1, \tag{65}$$

which is not at all illuminating at a first glance, as what does it mean from a physical point of view that the sum of the anti-correlation probabilities in different directions is greater than 1? We do not know how, or even attempt to answer to the latter question; we just point that we assumed the orientations $\mathbf{n}_1$, $\mathbf{n}_2$ and $\mathbf{n}_3$ to be arbitrary; in particular, if we choose the orientations such that they are trigonally symmetric[59], then a calculation in the framework of OQM similar in spirit to the one in [SN11, p.243-p.244] shows that

$$\sum_{1\leq i<j\leq 3} P\left(\left\{X^R_{\mathbf{n}_i} = X^R_{\mathbf{n}_j}\right\}\right) = \frac{3}{4}, \tag{66}$$

which is a clear violation of Bell's inequality (65).

We should pause our development and wonder what really happened. To answer to this, introduce the following statements:

$L =$ 'NISA between spacelike separated measurements of spin at SG-R and SG-L simply does not happen.'

$Q =$ 'OQM makes correct predictions.'

$P =$ 'The values of $X^{L,R}_{\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3}$ are preexisting.',

where we assumed without any further discussion that the way we reached (65), i.e. by means of simple properties derived from Kolmogorov's axioms of probability theory, is valid. In this subsection, we thus showed that

$$\begin{array}{r|l} 1 & Q \\ 2 & L \land Q \to P \\ 3 & Q \to \neg P \\ \hline 4 & Q \to \neg L \end{array}$$

where the validity of hypothesis 1 comes from experiments, hypothesis 2 is just pure reasoning about the concept of speed, and hypothesis 3 is Bell's argument; the conclusion follows from first-order predicate logic.

[59] By which we mean $\angle(\mathbf{n}_i, \mathbf{n}_j) = 2\pi/3$, for $i \neq j$, $i,j = 1, 2, 3$.

As now we are armed with a sound reason to affirm that OQM implies that NISA happens, we might take a step back and think whether the Nature itself insinuates that the latter is true, a hypothesis independent of any theory. Well, the convincing[60] experiment done by Alain Aspect et al. [ADR82] corroborates that an equivalent of (66) agrees with 'raw' data from Nature, so the statement Q in the Fitch diagram above can be replaced with

$$N = \text{'Nature is correct.'},$$

which is a tautology, yet at the same time slightly ambiguous, but leads the reader to the takeaway of this subsection:

Nature is such that non-informational superluminal action between spacelike separated events takes place.

Lastly, if the reader is wondering why in the case of the EPRB we have NISA and not ISA, where the latter means that one would be able to send a signal that travels back in time for some inertial observers, thus violating the principle of causality, we redirect her/him to [SN11, p.245].

[60] Up to loopholes.

2. Orthodox mathematical scattering theory

The Møller wave operators $\Omega_\pm$ emerge as a natural mathematical device in the study of scattering phenomena. In Subsections 2.1-2.5, we introduce their mathematical and physical properties, while in Subsection 2.6 we put them at use: we will connect an empirical quantity, the orthodox scattering cross section $\sigma_\psi^{\mathrm{OQM}}$, with the range of $\Omega_\pm$. Thus, we may infer that the wave operators are more than mere abstractions and find their legitimate place in our physical analysis; this motivates us to continue studying their properties in Section 4, this time in a 'Bohmian fashion'.

The background theory that we build in this section is based on the classical references [Tes14],[RS80],[RS79], and [Rud87], with selected key ideas from [Dol69],[Dol64],[Ens78], and [Coo57].

2.1. Incoming and outgoing asymptotic states

A particle in an initial state ψ is heading towards a target, where it interacts with forces. It is scattered off; its initial state ψ evolves under H, the full Hamiltonian. A detector is placed far away from the scattering center; the scattering potential is negligible in the surroundings of the detector. The particle hits the detector. What would the detector make of this particle?

Naturally, as the scattering potential is insignificant in the vicinity of the detector, the state of the particle should evolve like the one of a *free particle*. We can capture this with the following requirement:

$$\exists\ \psi_+ \text{ s.t. } \lim_{t\to+\infty} \|e^{-itH}\psi - e^{-itH_0}\psi_+\| = 0, \tag{67}$$

where ψ_+ is the $t = 0$ state of a freely moving particle.

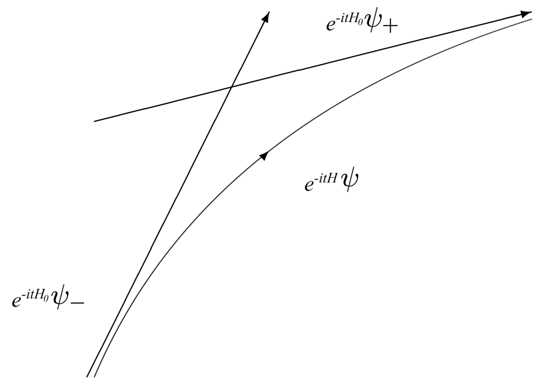

Figure 2: A schematic representation of the relationship between ψ and $\psi_\pm$. Based on [Tes14].

Similarly, as one goes to the limit $t \to -\infty$, we have that the particle should move as if no forces were present, as the scattering center is far away and there was no a priori contact with it. Then we can safely include the limit $t \to -\infty$ as a requirement as well, so extending the notation we simply get

$$\exists\ \psi_\pm \text{ s.t. } \lim_{t\to\pm\infty} \|e^{-itH}\psi - e^{-itH_0}\psi_\pm\| = 0. \tag{68}$$

It is useful to work further on the norm in (68). We arrive at:

$$\|e^{-itH}\psi - e^{-itH_0}\psi_\pm\| = \|\psi - e^{itH}e^{-itH_0}\psi_\pm\|, \tag{69}$$

where[61] we used $(e^{-itH})^* = e^{itH}$. From combining (68) with (69), i.e.

$$\exists\ \psi_\pm \text{ s.t. } \lim_{t\to\pm\infty} \|\psi - e^{itH}e^{-itH_0}\psi_\pm\| = 0, \tag{70}$$

we are now in the position to define the *Møller wave operators* $\Omega_\pm$ acting on

$$\left\{\psi_\pm \in L^2(\mathbb{R}^m) : \lim_{t\to\pm\infty} e^{itH}e^{-itH_0}\psi_\pm \text{ exists}\right\} =: \mathfrak{D}(\Omega_\pm) \tag{71}$$

via the limit

$$\Omega_\pm\psi_\pm = \lim_{t\to\pm\infty} e^{itH}e^{-itH_0}\psi_\pm, \tag{72}$$

where we use $\pm$ to label the general elements of (71) just to avoid introducing further notation.

Concisely, we thus have that

$$\Omega_\pm = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH}e^{-itH_0}. \tag{73}$$

We stress that the operators $\Omega_\pm$ are very natural constructs, as they are defined having in mind the following simple physical intuition: we look at each and every $\psi_\pm \in L^2(\mathbb{R}^m)$, and we check whether there is a corresponding $\psi \in L^2(\mathbb{R}^m)$ such that, when $\psi_\pm$ is evolved freely in the direction $t \to \pm\infty$ and ψ is evolved asymptotically in the same direction under the full Hamiltonian, we have that they are as similar as we please in the $L^2(\mathbb{R}^m)$ norm $\|\cdot\|$, such that the detector will not eventually be able to tell whether $\psi_\pm$ or ψ was the initial state. It then makes sense that $\Omega_\pm$ is the natural mapping $\psi_\pm \mapsto \psi$; it is well-defined as $\psi := \lim_{t\to\pm\infty} e^{itH}e^{-itH_0}\psi_\pm$, and limits are unique in a Hausdorff space, in particular[62] $L^2(\mathbb{R}^m)$. For further reference, we will call the normalized elements of

[61] Why not the equally valid $\|e^{-itH}\psi - e^{-itH_0}\psi_\pm\| = \|e^{itH_0}e^{-itH}\psi - \psi_\pm\|$? One might believe that continuing like this would lead to equivalent results, however there is a catch: see Subsection 2.4.

[62] In general, the inner product of a Hilbert space induces a norm $\|\cdot\| := \sqrt{\langle\cdot,\cdot\rangle}$ (the completeness of the Hilbert space being understood with respect to this induced norm). In turn, this norm induces a metric function on $L^2(\mathbb{R}^m) \times L^2(\mathbb{R}^m)$; it holds true that every metric space is Hausdorff, and that limits of sequences in a Hausdorff space are unique [Tes14, p.2-p.10].

$\mathfrak{D}(\Omega_\pm)$ *incoming/outgoing asymptotic states* (IOAS), while the normalized elements of $\mathfrak{R}(\Omega_\pm)$, the range of the wave operators, are simply *states that have IOAS.*

By construction, one has that $\Omega_\pm$ are bijective[63], hence invertible. Using a similar procedure to the one used to get (69), the inverses are given explicitly by

$$\Omega_\pm^{-1} = \underset{t\to\pm\infty}{\text{s-lim}}\, e^{itH_0}e^{-itH}.$$

Ultimately, the rationale for defining $\Omega_\pm$ lays in using them to shine a new light on the quantities appearing in scattering experiments; accordingly, in the next subsection we will talk about the *orthodox scattering cross section* $\sigma_\psi^{\mathrm{OQM}}$. However, *Dollard's scattering-into-cones theorem*, which provides a direct connection between the wave operators and scattering experiments, will be delayed to Subsection 2.6, as there are still many properties of $\Omega_\pm$ to be elucidated.

2.2. The orthodox scattering cross section

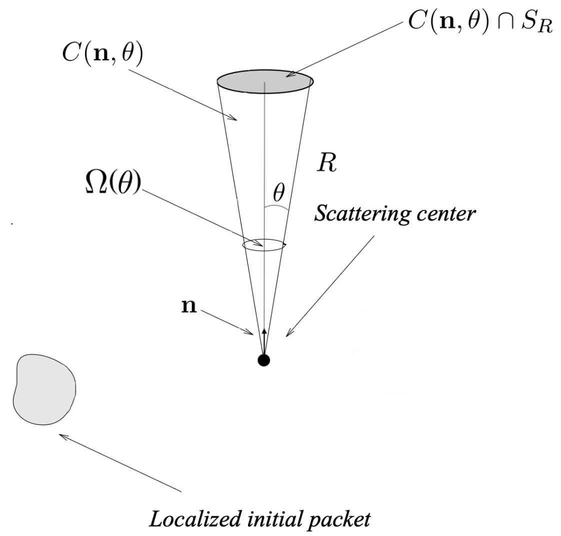

Figure 3: A scattering setup with the detector a spherical cap. Based on [DDGZ95a].

Back to the detector. We start to glimpse the theoretical importance of $\Omega_\pm$; all the same, we need to find a way to link them with the type of data collected by the detector. Suppose that we shoot at the scattering center one particle at a time with identical initial

[63]Since we restrict ourselves to the codomain $\mathfrak{R}(\Omega_\pm)$ as implied by the domain defined in (71) in order to have surjectivity, and by noting that injectivity is implied by the fact that $\|\psi - e^{itH}e^{-itH_0}\psi_\pm\| = \|e^{itH_0}e^{-itH}\psi - \psi_\pm\|$.

state ψ, waiting for each of them to get scattered off and to have enough time to reach and pass through the detector (or miss it). Consequently, we idealize our detector. We take it to be merely a spherical cap (see Figure 3) sliced from a sphere of radius R with origin in the scattering center: denote with θ its apex half-angle and with $\mathbf{R}$ the vector between the scattering center and the apex that satisfies $|\mathbf{R}| = R$, so that we can define the unit vector as $\mathbf{n} \coloneqq R^{-1}\mathbf{R}$.

For a large number of particles all prepared in the same initial state ψ, we record the number of times the detector is being hit, and divide it by the total number of particles. How can we get this quantity out of the theory? Well, it seems reasonable to note that #hits/#particles is getting closer and closer to the probability that the detector will be activated in a one-particle scattering experiment, as we increase the number of particles; this probability is given by

$$\sigma_{\psi}^{\text{OQM}}(\mathbf{n},\theta) \coloneqq \lim_{t\to\infty} \int_{C(\mathbf{n},\theta)} \left| e^{-itH}\psi(\mathbf{x}) \right|^2 d^m x, \tag{74}$$

where

$$C(\mathbf{n},\theta) \coloneqq \{\mathbf{x} \in \mathbb{R}^m : \mathbf{x}\cdot\mathbf{n} \geq |\mathbf{x}|\cos\theta\} \tag{75}$$

is a cone with the apex in the origin (scattering center), which intersected with $S_R \coloneqq \{\mathbf{x} \in \mathbb{R}^m : |\mathbf{x}| = R\}$, a sphere of radius R, gives the surface of the detector.

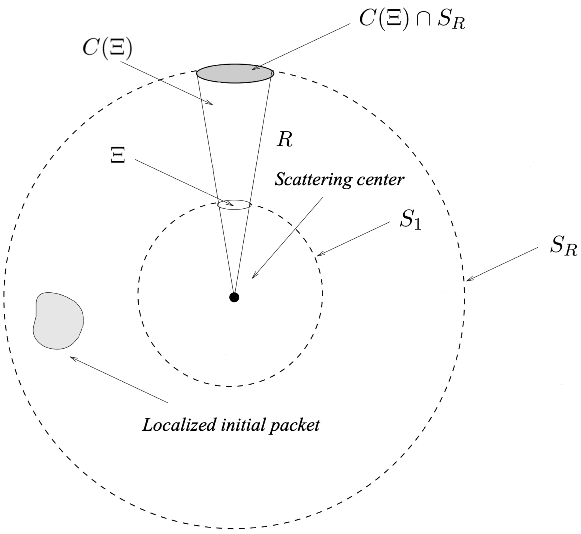

Figure 4: A scattering setup with the detector a sphere. From [DDGZ95a].

One can go further than (74) by noticing the simple connection between the solid angle Ω and the apex half-angle θ:

$$\Omega(\theta) = 4\pi\sin^2\left(\frac{\theta}{2}\right),$$

obtained via planar geometry, which hints that one might directly measure closed spherical caps of the unit sphere S_1, as they span the cone (75). Generalizing this intuition for an arbitrary set $\Xi \in \mathcal{B}(S_1)$, one can prove that the *orthodox scattering cross section*

$$\sigma_\psi^{\text{OQM}}(\Xi) := \lim_{t\to\infty} \int_{C(\Xi)} \left| e^{-itH}\psi(\mathbf{x}) \right|^2 d^m x, \tag{76}$$

with[64]

$$C(\Xi) := \left\{ c\mathbf{x} : c \in \mathbb{R}_0^+ \text{ and } \mathbf{x} \in \Xi \right\},$$

defines a measure in the scattering framework[65] we just discussed, as one can easily verify. And from now on we refer to S_R as the surface of the detector (see Figure 4), owing to the great flexibility of having a formula for the orthodox scattering cross section (76) for any $\Xi \in \mathcal{B}(S_1)$.

It happens that the measure σ_ψ^{OQM} is absolutely continuous with respect to the spherical measure[66] Ω; moreover, both are finite measures, in particular σ-finite, so the Radon-Nikodym derivative of σ_ψ^{OQM} exists, i.e. there exists a measurable function

$$h : (S_1, \mathcal{B}(S_1)) \longrightarrow (\mathbb{R}, \mathcal{B}(\mathbb{R}))$$

such that

$$\sigma_\psi^{\text{OQM}}(\Upsilon) = \int_\Upsilon h \, d\Omega,$$

where $\Upsilon \in \mathcal{B}(S_1)$. The standard notation for the Radon-Nikodym derivative h is

$$\frac{d\sigma_\psi^{\text{OQM}}}{d\Omega}, \tag{77}$$

and we call (77) the *differential cross section*, which is indeed the well-known quantity used in scattering experiments [RS79, p.14-p.15].

Nevertheless, we stress that (77) might not exist in a more general scattering setup, as pointed in [RS79, p.15], and as we strive for generality, we will instead focus on the properties of (76). Nothing is lost here from a physical point of view, as going from (76) to (77) is just a mathematical procedure.

[64] In general, for an arbitrary $n \in \mathbb{N}$, the cone $C_n(\Xi) := \{c\mathbf{x} : c \in [0, n] \text{ and } \mathbf{x} \in \Xi\}$ is Lebesgue measurable, as can be easily shown, hence also $\bigcup_{i=1}^\infty C_n(\Xi) = C(\Xi)$ is Lebesgue measurable.

[65] For a definition of the scattering cross section in a more general setting, the reader might want to consult [RS79, p.14-p.15].

[66] One should take notice that Ω does equate the 'area' of a generalized spherical cap Ξ with $\mathbf{m}$ times the 'volume' of the generalized unit cone $C_1(\Xi) := \{c\mathbf{x} : c \in [0, 1] \text{ and } \mathbf{x} \in \Xi\}$, the multiplication by the dimension m being such that $\Omega(S_1)$ will be the surface area of the m-sphere, as it is explained in [Sch06, p.14]. Therefore, for $\Xi \in \mathcal{B}(S_1)$ such that $\Omega(\Xi) = 0$, we also have that $\lambda(C_1(\Xi)) = 0$, and as $\lambda(C_n(\Xi)) = n^m \lambda(C_1(\Xi)) = 0$ for any $n \in \mathbb{N}$, it also follows that $\lambda\left(\bigcup_{i=1}^\infty C_i(\Xi)\right) = \lambda(C(\Xi)) = 0$, so obviously $\sigma_\psi^{\text{OQM}}(\Xi) = 0$ as well, as we take the limit of a quantity obtained by integrating over a set of Lebesgue measure zero, which should then be equal to zero.

2.3. The properties of the Möller wave operators

A quick glance at (71) indicates possible trouble. More precisely, could it be that $\mathfrak{D}(\Omega_\pm) = \{0_{L^2}\}$? Is this happening only for some 'strange' potentials V that do not pose any physical significance, or is it the case that $\Omega_\pm$ fail to exist[67] even for realistic situations?

To answer this question, let us take the simplest potential possible, $V =$ 'nonzero constant'. In this case it is instructive to calculate directly

$$\begin{aligned}
\left\|\psi_1 - e^{itH}e^{-itH_0}\psi_2\right\| &= \left\|\psi_1 - e^{iVt}\psi_2\right\| \\
&= \int_{\mathbb{R}^m} \left|\psi_1(\mathbf{x}) - e^{iVt}\psi_2(\mathbf{x})\right|^2 \, d^m x \\
&= \int_{\mathbb{R}^m} \left|a_1(\mathbf{x}) + ib_1(\mathbf{x}) - e^{iVt}(a_2(\mathbf{x}) + ib_2(\mathbf{x}))\right|^2 \, d^m x \\
&= \sum_{i=1}^{2} \int_{\mathbb{R}^m} (a_i^2(\mathbf{x}) + b_i^2(\mathbf{x}))\, d^m x \\
&+ \sin(Vt) \int_{\mathbb{R}^m} (2a_1(\mathbf{x})b_2(\mathbf{x}) - 2a_2(\mathbf{x})b_1(\mathbf{x})) \, d^m x \\
&- \cos(Vt) \int_{\mathbb{R}^m} (2b_1(\mathbf{x})b_2(\mathbf{x}) + 2a_1(\mathbf{x})a_2(\mathbf{x}))\, d^m x,
\end{aligned} \tag{78}$$

for arbitrary $\psi_i \in L^2(\mathbb{R}^m)$ with $\mathrm{Re}\{\psi_i\} = a_i$, $\mathrm{Im}\{\phi_i\} = b_i$, $i = 1, 2$.

Note that the limit $t \to \pm\infty$ of the norm in the left-hand side of the first line of (78) does not exist, as the existence of the limit of the norm would be equivalent with the existence of the limits[68] $\lim_{t\to\pm\infty} \sin(Vt)$ and $\lim_{t\to\pm\infty} \cos(Vt)$; the latter statement is obviously not true. In particular, the limit that defines $\mathfrak{D}(\Omega_\pm)$, which is of shape (78), does not exist for $\psi \neq 0_{L^2}$, so $\mathfrak{D}(\Omega_\pm) = \{0_{L^2}\}$.

This looks downright worrying: if our wave operators cannot accommodate such a banal potential, then what are they good for? Of course that one can always shift the zero energy axis such that $V = 0$, and then the problem is virtually solved, as then we have $\Omega_\pm = \mathbb{I}$.

The takeaway of the previous paragraph is that the Møller wave operators might not exist for fairly 'normal' potentials, although it is fair to reassure the reader that the case of a constant nonzero potential is more of a mathematical technicality rather than a flaw in our physical reasoning. We will return in the next subsection with a criterion for the existence of $\Omega_\pm$ in the scattering regime we introduced in Subsection 2.1; all the same,

[67] When we say that the wave operators $\Omega_\pm$ exist, we simply mean that they are nontrivial, i.e. $\mathfrak{D}(\Omega_\pm) \neq \{0_{L^2}\}$.

[68] As $\psi_i \in L^2(\mathbb{R}^m)$, then a_i, $b_i \in L^2(\mathbb{R}^m)$ as well, so a_ib_j, a_ia_j, $b_ib_j \in L^1(\mathbb{R}^m)$, for $i \neq j$, $i = 1, 2$ and $j = 1, 2$; we then have that the right-hand side of (78) is finite.

for the rest of this subsection we will assume that $\mathfrak{D}(\Omega_\pm) \neq \{0_{L^2}\}$ and carry on with proving their properties.

Looking once again at (72), and exploiting the fact that the limit of the norm is the norm of the limit (as the norm is continuous), we can see that

$$\|\Omega_\pm \psi\| = \lim_{t\to\pm\infty} \|e^{itH}e^{-itH_0}\psi\| = \lim_{t\to\pm\infty} \|\psi\| = \|\psi\|$$

proves that the wave operators are isometries[69] by construction, and via the definition of $\Omega_\pm$, we also have surjectivity: in a word, they are unitary. We emphasize that these properties are independent of the choice of V.

To boot, take a sequence $\psi_\pm^n \to \psi_\pm$ as $n \to \infty$, where $\{\psi_\pm^n\}_{n=1}^\infty \subseteq \mathfrak{D}(\Omega_\pm)$. For a fixed n^* and $\psi_{n^*} \coloneqq \lim_{t\to\pm\infty} e^{itH}e^{-itH_0}\psi_\pm^{n^*}$, the triangle inequality implies

$$\begin{aligned}\|\psi - e^{itH}e^{-itH_0}\psi_\pm\| \leq & \|\psi - \psi_{n^*}\| + \|e^{itH}e^{-itH_0}(\psi_\pm^{n^*} - \psi_\pm)\| + \\ & + \|\psi_{n^*} - e^{itH}e^{-itH_0}\psi_\pm^{n^*}\| \\ = & \|\psi - \psi_{n^*}\| + \|\psi_\pm - \psi_\pm^{n^*}\| + \|\psi_{n^*} - e^{itH}e^{-itH_0}\psi_\pm^{n^*}\|,\end{aligned} \tag{79}$$

where in turn[70] $\psi \coloneqq \lim_{n\to\infty}\psi_n$. In the limit $t \to \pm\infty$, (79) becomes

$$\lim_{t\to\pm\infty} \|\psi - e^{itH}e^{-itH_0}\psi_\pm\| \leq \|\psi - \psi_{n^*}\| + \|\psi_\pm - \psi_\pm^{n^*}\|. \tag{80}$$

But n^* is just a dummy variable, so by sending $n^* \to \pm\infty$ in (80), we see that

$$\lim_{t\to\pm\infty} \|\psi - e^{itH}e^{-itH_0}\psi_\pm\| = 0, \tag{81}$$

which means that $\psi \in \mathfrak{D}(\Omega_\pm)$. Thus we just showed that $\mathfrak{D}(\Omega_\pm)$ is closed in $L^2(\mathbb{R}^m)$, and as $\left(\Omega_\pm^{-1}\right)^{-1} = \Omega_\pm$ and $\Omega_\pm^{-1}$ is continuous, the wave operators take $\mathfrak{D}(\Omega_\pm)$ to another closed set of $L^2(\mathbb{R}^m)$, which is by definition $\mathfrak{R}(\Omega_\pm)$.

Other properties that are independent of V can be obtained by observing that, for a fixed and arbitrary $t' \in \mathbb{R}$, $\psi \in \mathfrak{D}(\Omega_\pm)$, we can rewrite

$$\lim_{t\to\pm\infty} e^{itH}e^{-itH_0}e^{-it'H_0}\psi = \lim_{t\to\pm\infty} e^{-it'H}e^{i(t'+t)H}e^{-i(t+t')H_0}\psi,$$

which is via the definition of $\Omega_\pm$ equivalent to

$$\Omega_\pm e^{-it'H_0}\psi = e^{-it'H}\Omega_\pm\psi, \tag{82}$$

where for both we used properties from Lemma A.2.

[69] In particular continuous and injective.

[70] The limit $n \to \infty$ exists as $\{\psi_n\}_{n=1}^\infty$ is a Cauchy sequence in the Hilbert space $L^2(\mathbb{R}^m)$, therefore it converges by completeness.

The equality (82) implies directly that $\mathfrak{D}(\Omega_\pm)$ is invariant under $e^{-it'H_0}$, and likewise $e^{-it'H}$ leaves $\mathfrak{R}(\Omega_\pm)$ invariant, for an arbitrary $t' \in \mathbb{R}$. Besides, the corresponding invariance extends also to the orthogonal spaces, as it follows for $\psi \in \mathfrak{D}(\Omega_\pm)$ and $\psi^\perp \in \mathfrak{D}(\Omega_\pm)^\perp$ that

$$\langle e^{-it'H_0}\psi^\perp, \psi\rangle = \langle \psi^\perp, e^{it'H_0}\psi\rangle = 0, \tag{83}$$

as $e^{it'H_0}\psi \in \mathfrak{D}(\Omega_\pm)$ from (82). Then (83) mandates that $\mathfrak{D}\left(\Omega_\pm\right)^\perp$ is invariant under $e^{-it'H_0}$, and similarly it can be shown that $\mathfrak{R}\left(\Omega_\pm\right)^\perp$ is invariant under $e^{-it'H}$.

In the next step, to get an identity involving the wave operators and directly H, H_0, we strongly differentiate (see (187) and the background remarks) (82) to get

$$\Omega_\pm \left.\frac{d}{dt'}e^{-it'H_0}\right|_{t'=0}\psi = \left.\frac{d}{dt'}e^{-it'H}\right|_{t'=0}\Omega_\pm\psi,$$

which turns into

$$\Omega_\pm H_0\psi = H\Omega_\pm\psi,$$

for $\psi \in \mathfrak{D}(H_0) \cap \mathfrak{D}(\Omega_\pm)$, the above identity being known as the *intertwining property.*

We stop here with our development, as we cannot do much more in the absence of supplementary information regarding V. For further use, we collect all the properties that we proved in a compact lemma:

Lemma 2.1. *For $\Omega_\pm$ defined as in (73) it holds true that:*

1. $\|\Omega_\pm\psi\| = \|\psi\|$ *and* $\mathfrak{D}(\Omega_\pm) \longleftrightarrow \mathfrak{R}(\Omega_\pm)$.
2. $\mathfrak{D}(\Omega_\pm)$, $\mathfrak{R}(\Omega_\pm)$ *are closed in* $L^2(\mathbb{R}^m)$.
3. $e^{-itH_0}\mathfrak{D}(\Omega_\pm) \subseteq \mathfrak{D}(\Omega_\pm)$.
4. $e^{-itH_0}\mathfrak{D}(\Omega_\pm)^\perp \subseteq \mathfrak{D}(\Omega_\pm)^\perp$.
5. $e^{-itH}\mathfrak{R}(\Omega_\pm) \subseteq \mathfrak{R}(\Omega_\pm)$.
6. $e^{-itH}\mathfrak{R}(\Omega_\pm)^\perp \subseteq \mathfrak{R}(\Omega_\pm)^\perp$.
7. $\Omega_\pm H_0 = H\Omega_\pm$ *on* $\mathfrak{D}(H_0) \cap \mathfrak{D}(\Omega_\pm)$.

In 3.-6., $t \in \mathbb{R}$ is arbitrary.

2.4. The existence of incoming and outgoing asymptotic states

Assume[71] $\mathfrak{D}(H_0) \subseteq \mathfrak{D}(H)$, and denote $Y(t) := e^{itH}e^{-itH_0}\psi$, where $\psi \in \mathfrak{D}(H_0)$. In the case that $\lim_{t\to\pm\infty} Y(t)$ exists, we have that $\psi \in \mathfrak{D}(\Omega_\pm)$; for this to happen, the

[71] This domain condition is just a technical requirement to ensure that taking the derivative of $e^{itH}e^{-itH_0}\psi$ is well-defined, as it is stipulated in [Tes14, p.146].

completeness of $L^2(\mathbb{R}^m)$ implies that it is necessary and sufficient to show that it is Cauchy, i.e.

$$\lim_{t_1,t_2\to\pm\infty} \|Y(t_1) - Y(t_2)\| = 0.$$

But where is the potential V? Lurking inside e^{itH}! We can expose it with a trick similar to the one we used to derive the intertwining property (see Corollary A.2.1):

$$Y'(t) = ie^{itH}(H - H_0)e^{-itH_0}\psi = ie^{itH}Ve^{-itH_0}\psi,$$

so

$$Y(t_1) - Y(t_2) = \int_{t_1}^{t_2} Y'(t)\, dt = \int_{t_1}^{t_2} ie^{itH}Ve^{-itH_0}\psi\, dt, \tag{84}$$

these manipulations being allowed firstly by the fact that $t \mapsto Y(t)$ is differentiable in the sense of (187), and secondly we have that $Y'(t)$ is continuous as it follows from an application of Lemma A.2, hence integrable.

We then simply see from (84) that

$$\|Y(t_1) - Y(t_2)\| = \left\|\int_{t_1}^{t_2} ie^{itH}Ve^{-itH_0}\psi\, dt\right\| \leq \int_{t_1}^{t_2} \|Ve^{-itH_0}\psi\|\, dt, \tag{85}$$

where we assumed without loss of generality that $0 \leq t_1 < t_2$, as we now focus on the case $t_1, t_2 \to \infty$. A plausible strategy to prove that $\lim_{t_1,t_2\to\infty} \|Y(t_1) - Y(t_2)\| = 0$ using the estimate (85) would be to have a V for which

$$\int_0^\infty \|Ve^{-itH_0}\psi\|\, dt < \infty, \tag{86}$$

as then by sending $t_2 \to +\infty$ firstly, the right-hand side of (85) is finite as well, as it is lesser or equal to the left-hand side of (86); we can then send $t_1 \to +\infty$, thus the norm on the left of (85) becomes null, which is equivalent to the existence of $\lim_{t\to+\infty} Y(t) = \Omega_+\psi$. In the case $t_1, t_2 \to -\infty$, the proof goes the same way, but now (86) reads

$$\int_0^\infty \|Ve^{+itH_0}\psi\|\, dt < \infty;$$

thus, for $\Omega_\pm$, we require

$$\int_0^\infty \|Ve^{\mp itH_0}\psi\|\, dt < \infty. \tag{87}$$

What we just proved is one of the many variants of Cook's method that appear in the literature. It gives us the piece of mind that $\Omega_\pm$ exists, provided that our potential V obeys (87). It also provides us with an upper bound for the difference between an IOAS ψ and a state that has an IOAS $\Omega_\pm\psi$, as one can see from (85) by setting $t_1 = 0$ and sending $t_2 \to \pm\infty$. For the sake of conciseness, we formulate the theorem:

Theorem 2.2 (Cook's method)**.** *Let V be such that $\mathfrak{D}(H_0) \subseteq \mathfrak{D}(H)$. If we also have that (87) holds true for a $\psi \in \mathfrak{D}(H_0)$, then $\psi \in \mathfrak{D}(\Omega_\pm)$. Moreover, the difference between an IOAS and a state that has an IOAS is bounded from above, i.e.*

$$\|(\Omega_\pm - \mathbb{I})\psi\| \leq \int_0^\infty \|Ve^{\mp itH_0}\psi\|\, dt. \tag{88}$$

The right-hand side of (88) is certainly an informative upper bound, as it depends on V. In order to put to use Cook's method, we go back to Kato's criterion for self-adjointness (as presented in Appendix B). Let us find a V that satisfies (190) and (87) simultaneously.

Easily enough, if we impose that $V \in L^2(\mathbb{R}^m)$, then all the requirements of Theorem B.1 are met; this implies that we can take $\mathfrak{D}(H_0) = \mathfrak{D}(H)$, so the domain condition of Cook's method is satisfied. To prove that for square-integrable potentials (85) is true, we calculate for the integrand

$$\|Ve^{-itH_0}\psi\| \leq \|e^{-itH_0}\psi\|_\infty \|V\| \leq \frac{1}{|4\pi t|^{m/2}}\, \|\psi\|_{L^1}\, \|V\| < \infty, \tag{89}$$

where we used Lemma C.1 in (89), for $\psi \in L^1(\mathbb{R}^m) \cap L^2(\mathbb{R}^m)$ and $t \neq 0$. Integrating over the positive functions in (89), one obtains

$$\int_1^\infty \|Ve^{-itH_0}\psi\|\, dt \leq \frac{2}{(4\pi)^{m/2}(m-2)}\, \|\psi\|_{L^1}\, \|V\| < \infty,$$

which ensures that (86) is true, for $m \geq 3$.

Insofar, we managed to show that if $\psi \in L^1(\mathbb{R}^m) \cap L^2(\mathbb{R}^m)$, then $\psi \in \mathfrak{D}(\Omega_\pm)$. This seems rather artificial, but a simple ϵ-δ argument shows that $L^1(\mathbb{R}^m) \cap L^2(\mathbb{R}^m)$ is dense in $L^2(\mathbb{R}^m)$, and moreover as $\|e^{itH}e^{-itH_0}\|_o = 1$, for any $t \in \mathbb{R}$, by a standard property[72] we have that $\mathfrak{D}(\Omega_\pm) = L^2(\mathbb{R}^m)$. This agrees with our physical intuition, as roughly speaking the fact that $V \in L^2(\mathbb{R}^m)$ suggests[73] a certain sense of decay at large $\mathbf{x}$, so a scattered particle with any initial state ψ should move quasi-freely after a long period of time, hence it admits IOAS.

But what about $\mathfrak{R}(\Omega_+)$ and $\mathfrak{R}(\Omega_-)$? They certainly are nonempty, yet trivial if $\mathfrak{D}(\Omega_\pm) = \{0_{L^2}\}$; what can we say about $\mathfrak{R}(\Omega_+) \stackrel{?}{=} \mathfrak{R}(\Omega_-)$ instead? The intuition tells us that they should be equal, but unfortunately trying to adapt Cook's method to $\Omega_\pm^{-1}$ is doomed to failure in most of the cases, as then in the left-hand side of (88) H_0 is replaced by H, and consequently bounding the integrand $\|Ve^{\mp itH}\psi\|$ as in (89) is a daunting

[72]Suppose that $A_n \in L(\mathfrak{H})$ is a sequence of bounded operators that satisfies $A_n\psi \to A\psi$ for ψ in a dense set of $\mathfrak{H}$, and moreover $\exists C > 0$ such that $\|A_n\| \leq C$, for any n. Then $\text{s-lim}_{n\to\infty} A_n = A$.

[73]For example, the Coulomb potential is not square-integrable. Additionally, in the case of a particle living on the real axis, for which we take $\mathfrak{H} := L^2(\mathbb{R})$, and besides $\psi \in L^2(\mathbb{R})$, we also assume that $d\psi/\,dx \in L^2(\mathbb{R})$, then $\lim_{x\to\pm\infty} \psi(x) = 0$, according to [DT09, p.267-p.268].

task, as we do not have a formula similar to (193) for e^{-itH}. However, Tosio Kato and Sigekatu Kuroda [KK59] showed that, if besides V square-integrable we also assume that it is integrable, then the states that have IAS also have OAS, and vice versa, i.e. $\mathfrak{R}(\Omega_+) = \mathfrak{R}(\Omega_-)$.

Lemma 2.3. *For $V \in L^2(\mathbb{R}^m)$, we have that*

1. $H = H^*$.
2. $\mathfrak{D}(H_0) = \mathfrak{D}(H)$.
3. $\mathfrak{D}(\Omega_\pm) = L^2(\mathbb{R}^m)$.

Moreover, if one has that $V \in L^1(\mathbb{R}^m) \cap L^2(\mathbb{R}^m)$, then also:

4. $\mathfrak{R}(\Omega_+) = \mathfrak{R}(\Omega_-)$.

Whenever $\mathfrak{R}(\Omega_+) = \mathfrak{R}(\Omega_-)$ is true, we will refer to the states that have IOAS as being elements of $\mathfrak{R}(\Omega) := \mathfrak{R}(\Omega_+) = \mathfrak{R}(\Omega_-)$. For the remainder of this section, we will restrict ourselves to potentials $V \in L^1(\mathbb{R}^m) \cap L^2(\mathbb{R}^m)$, for which all the properties presented in Lemma 2.3 are true.

2.5. Asymptotic completeness via Enss' method

All seems well if $\mathfrak{D}(\Omega_\pm) \neq \{0_{L^2}\}$, but what can we say about $\mathfrak{R}(\Omega)$? Would it be reasonable to expect that $\mathfrak{R}(\Omega) = L^2(\mathbb{R}^m)$ for any V, or are there some potentials strong enough to 'capture' the particle and prevent it to leave the scattering region?

Given our familiarity with the *bound states* of the electrons of, say, a hydrogen-like atom, we might be inclined to expect that some elements of $L^2(\mathbb{R}^m)$ will not make it to $\mathfrak{R}(\Omega)$. But these are just suppositions unless we quantify the meaning of 'bound states'; for a start, we said that they are not the elements of $\mathfrak{R}(\Omega)$, which are states that have both IAS and OAS, so we can naturally refer to them as *scattering states*. Consequently, by contrasting them with the scattering states, the bound states should be such that they remain localized in a bounded subset of $\mathbb{R}^m$ for all times. It was David Ruelle who showed[74] the following: there exists a compact H-dependent set[75] $\mathfrak{H}_{\text{bnd}}(H) \subseteq L^2(\mathbb{R}^m)$

[74] In [Rue69]. For the explicit conditions he imposed on V, as well as on the domain of H, see [Rue69, p.656-657].

[75] From physics, we know that the eigenvectors of H correspond to 'bound states'. Thus, Ruelle took the span of the eigenvectors of H (i.e. the span of all the solutions of the time-independent Schrödinger equation (176)) as a candidate set for those whose elements have the property (90), which turned out to be a correct guess.

such that $\psi \in \mathfrak{H}_{\text{bnd}}(H)$ is equivalent to it being conceptually a bound state, in the sense that for any $\varepsilon > 0$, there is an $R > 0$ such that

$$\sup_{t\in\mathbb{R}} \int_{\overline{B_R^c}} |e^{-itH}\psi(\mathbf{x})|^2 \, d^m x < \varepsilon, \tag{90}$$

while for a $\psi \in \mathfrak{H}_{\text{bnd}}(H)^\perp =: \mathfrak{H}_{\text{sct}}(H)$, it is true for any $R > 0$ that

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \int_{B_R} |e^{-itH}\psi(\mathbf{x})|^2 \, d^m x \, dt = 0. \tag{91}$$

Using a basic property of Hilbert spaces [Tes14, p.59], we can then express our underlying Hilbert space $L^2(\mathbb{R}^m)$ as

$$L^2(\mathbb{R}^m) = \mathfrak{H}_{\text{bnd}}(H) \oplus \mathfrak{H}_{\text{sct}}(H). \tag{92}$$

We are thus left to link $\mathfrak{R}(\Omega)$ with $\mathfrak{H}_{\text{bnd}}(H)$ and $\mathfrak{H}_{\text{sct}}(H)$, respectively. For this feat, we get inspired from the decomposition (92): as $\mathfrak{H}_{\text{bnd}}(H)$ and $\mathfrak{H}_{\text{sct}}(H)$ help us to express $L^2(\mathbb{R}^m)$ as a direct sum, could it be the case that we can find another (of course H-dependent) direct sum decomposition for $L^2(\mathbb{R}^m)$, this time using a more 'mathematical' approach?

Take the linear space of continuous complex-valued functions[76] $C(\sigma(H))$, and observe that the functional

$$f \mapsto \langle \psi, f(H)\psi \rangle$$

for $f \in C(\sigma(H))$, is bounded, linear and positive[77], where $f(H)$ is as prescribed by the functional calculus introduced in Appendix A; hence the Riesz-Markov-Kakutani representation theorem[78] guarantees that there exists a unique ψ, H-dependent measure

$$\mu_H^\psi : \mathcal{B}(\sigma(H)) \longrightarrow \mathbb{R}_0^+$$

such that

$$\langle \psi, f(H)\psi \rangle = \int_{\sigma(H)} f(\lambda) \, d\mu_H^\psi, \tag{93}$$

and we call μ_H^ψ the *spectral measure*[79] (as (93) represents another variant of the spectral theorem [DT09, p.320]). In what follows, we will suppress the H subscript, as the notation gets cluttered, but the reader should bear in mind that the spectral measure $\mu_H^\psi \equiv \mu^\psi$ is H-dependent as well.

---

[76]As H is self-adjoint, we have that $\sigma(H) \subseteq \mathbb{R}$; additionally, $\sigma(H)$ is closed.

[77]In the sense that for $f \geq 0$, we have that $\langle \psi, f(H)\psi \rangle \geq 0$.

[78]Its conditions are stated in [Lan93, p.264]; we just mention here that $\mathbb{R}$ is trivially locally compact, and $\sigma(H) \subseteq \mathbb{R}$ is closed, so we have that $\sigma(H)$ is locally compact as well.

[79]It comes with the nice feature of being *regular*, in the sense that for $K \in \mathcal{B}(\sigma(H))$ a compact set, we have that $\mu_H^\psi(K) < \infty$.

Now, a variant of the Lebesgue decomposition theorem [RS80, p.22-p.23] gives the following decomposition for the spectral measure:

$$\mu^\psi = \mu^\psi_{\mathrm{pp}} + \mu^\psi_{\mathrm{ac}} + \mu^\psi_{\mathrm{sc}},$$

where μ^ψ_{pp} is a *pure point measure*[80], μ^ψ_{ac} is an *absolutely continuous measure*, with the same meaning as in Subsection 2.2, and finally the measure μ^ψ_{sc} is *singularly continuous*[81]. Consequently, it then comes natural to define:

$$\mathfrak{H}_{\mathrm{xx}}(H) := \{\psi \in L^2(\mathbb{R}^m) : \mu^\psi = \mu^\psi_{\mathrm{xx}}\},$$

with indices $\mathrm{xx} \in \{\mathrm{pp}, \mathrm{ac}, \mathrm{sc}\}$, such that we can now write[82] (see also [Tes14, p.118])

$$L^2(\mathbb{R}^m) = \mathfrak{H}_{\mathrm{pp}}(H) \oplus \mathfrak{H}_{\mathrm{ac}}(H) \oplus \mathfrak{H}_{\mathrm{sc}}(H).$$

As it can be seen, we obtained another decomposition for $L^2(\mathbb{R}^m)$; we recall the other decomposition, the one consisting of the physically meaningful $\mathfrak{H}_{\mathrm{bnd}}(H)$ and $\mathfrak{H}_{\mathrm{sct}}(H)$. The link between them is straightforward: Ruelle identifies $\mathfrak{H}_{\mathrm{bnd}}(H)$ with $\mathfrak{H}_{\mathrm{pp}}(H)$ in the article [Rue69]. Accordingly, $\mathfrak{H}_{\mathrm{sct}}(H) = \mathfrak{H}_{\mathrm{ac}}(H) \oplus \mathfrak{H}_{\mathrm{sc}}(H)$, so that we can say that the elements of $\mathfrak{H}_{\mathrm{xx}}(H)$, for $\mathrm{xx} \in \{\mathrm{ac}, \mathrm{sc}\}$, satisfy (91), i.e. 'leave in the time-mean any finite region of space', in the words of Volker Enss [Ens78].

To boot, the intertwining property presented in Lemma 2.1 implies that

$$\Omega_\pm^{-1} H \Omega_\pm \psi = H_0 \psi,$$

where $\psi \in \mathfrak{D}(\Omega_\pm) \cap \mathfrak{D}(H_0)$. Hence $H|_{\mathfrak{R}(\Omega)}$ is unitarily equivalent[83] with H_0, so we have the useful a priori result

$$\mathfrak{R}(\Omega) \subseteq \mathfrak{H}_{\mathrm{ac}}(H),$$

which is fully justified in [His12].

Thus, finally, *completeness* of the wave operators means proving that

$$\mathfrak{H}_{\mathrm{ac}}(H) \subseteq \mathfrak{R}(\Omega)$$

as well, so that, with the a priori result we just mentioned, we have that $\mathfrak{R}(\Omega) = \mathfrak{H}_{\mathrm{ac}}(H)$, while by their *asymptotic completeness* we refer to the validity of the extra condition $\mathfrak{H}_{\mathrm{sc}}(H) = \emptyset$.

[80] By which we mean that $\mu^\psi_{\mathrm{pp}}(S) = \sum_{s \in S} \mu^\psi_{\mathrm{pp}}(\{s\})$ (singletons are closed sets, hence Borel measurable, in any Hausdorff space), for any $S \in \mathcal{B}(\sigma(H))$.

[81] I.e. μ^ψ_{sc} is continuous as for all $x \in \sigma(H)$, we have that $\mu^\psi_{\mathrm{sc}}(\{x\}) = 0$, and it is singular with respect to the Lebesgue measure λ as there exists a set $S \in \mathcal{B}(\sigma(H))$ such that $\mu^\psi_{\mathrm{sc}}(S) = 0$, and $\lambda(\sigma(H) \setminus S) = 0$.

[82] Assuming that neither of them are the empty set; if one (or two) turns out to be empty, then the decomposition is formed by taking the direct sum of the remaining one(s).

[83] As $(\Omega_\pm)^* = \Omega_\pm^{-1}$ on $\mathfrak{R}(\Omega)$.

The literature abounds with ways to choose V for which $\Omega_\pm$ are asymptotically complete: for very general conditions imposed on V, the reader might be interested in reading [Teu99, p.22].

It is worth noting that this characterization of the dynamical properties of a $\psi \in L^2(\mathbb{R}^m)$ in terms of the sets $\mathfrak{H}_{\mathrm{xx}}(H)$ (i.e. proving asymptotic completeness) spares us of checking (90) and (91) directly; it is known by the name of *Enss' (geometrical) method*, firstly introduced in [Ens78].

We lastly mention that, from the point of view of spectra, we have the decomposition

$$\sigma(H) = \sigma_{\mathrm{pp}}(H) \cup \sigma_{\mathrm{ac}}(H) \cup \sigma_{\mathrm{sc}}(H),$$

where

$$\sigma_{\mathrm{xx}}(H) = \sigma\left(H|_{\mathfrak{H}_{\mathrm{xx}}}\right), \tag{94}$$

again with indices $\mathrm{xx} \in \{\mathrm{pp}, \mathrm{ac}, \mathrm{sc}\}$ (for notational convenience, we suppressed the H-dependence of $\mathfrak{H}_{\mathrm{xx}}(H)$ in (94)). It can be shown easily that the eigenvalue of any solution of (176), i.e. an eigenvector of H, is an element of[84] σ_{pp}, as one expects.

2.6. Dollard's scattering-into-cones theorem

In (76), we defined the scattering cross section $\sigma_\psi^{\mathrm{OQM}}$ for a generalized cone $C(\Xi)$ generated by a set $\Xi \in \mathcal{B}(S_1)$. However, the right-hand side of (76) is 'raw', in the sense that it will prove useful to work further on the defining expression of $\sigma_\psi^{\mathrm{OQM}}$ in order to find alternative formulae that might be linked with $\Omega_\pm$, which we believe at this point are quite fundamental for scattering theory; by pursuing this line of action, we will also get rid of the pesky limit in (76).

With this goal in mind, for an arbitrary initial state $\psi \in \mathfrak{R}(\Omega)$, as $\mathfrak{D}(\Omega_\pm) = L^2(\mathbb{R}^m)$, we have that $\exists$ IAS ψ_+, OAS ψ_- in $L^2(\mathbb{R}^m)$ such that $\psi = \Omega_+\psi_+ = \Omega_-\psi_-$. Picking one of them, e.g. $\psi = \Omega_+\psi_+$, the connection to the left-hand side of (76) is straightforward. Consequently, for the right-hand side of (76) in the free case, Lemma D.2 and D.3 immediately imply that[85]

$$\begin{aligned} \sigma_{\psi,\mathrm{free}}^{\mathrm{OQM}}(\Xi) &= \lim_{t\to\pm\infty} \int_{C(\Xi)} \left|e^{-itH_0}\psi(\mathbf{x})\right|^2 \, d^m x \\ &= \lim_{t\to\pm\infty} \int_{C(\Xi)} \left|(C_t\psi)(\mathbf{x})\right|^2 \, d^m x \\ &= \lim_{t\to\pm\infty} (2t)^{-m} \int_{C(\Xi)} \left|(\mathcal{F}\psi)(\mathbf{x}/2t)\right|^2 \, d^m x, \end{aligned} \tag{95}$$

[84] But mind the fact that σ_{pp} is often larger than its subset consisting of the eigenvalues of H!

[85] We will continue our development for $t \to \pm\infty$ and identify $\sigma_\psi^{\mathrm{OQM}}$ with $t \to -\infty$ as well, as there is no difference between the two from a mathematical point of view.

so by conveniently introducing

$$- C(\Xi) \coloneqq \{-\mathbf{x} : \mathbf{x} \in C(\Xi)\} ,$$

the change of variables[86] $\mathbf{k} = \mathbf{x}/2t$ brings (95) to

$$\lim_{t\to\pm\infty} \int_{C(\Xi)} \left|e^{-itH_0}\psi(\mathbf{x})\right|^2 d^m x = \int_{\pm C(\Xi)} |(\mathcal{F}\psi)(\mathbf{k})|^2 \, d^m k, \tag{96}$$

as $\pm\frac{1}{2t}C(\Xi) = \pm C(\Xi)$, and where it is worth noting that there is no time-dependence on the right-hand side.

The result (96) has also an interesting physical interpretation: for a **classical** particle[87] moving with constant velocity $2\mathbf{p}$ and starting at $\mathbf{x}(0) = \mathbf{x}_0$, its trajectory is simply prescribed by the equation $\mathbf{x}(t) = \mathbf{x}_0 + 2\mathbf{p}t$, so $\mathbf{x}(t)/2t = \mathbf{x}_0/2t + \mathbf{p} \approx \mathbf{p}$ asymptotically. In consequence, $|(\mathcal{F}\psi)(\mathbf{k})|^2$ can be interpreted as a pdf[88]. Heuristically, we have then for large t that the probability that the position of the free particle is in the Borel measurable $\Upsilon \subseteq \mathbb{R}^m$ is equal to the probability of finding its momentum in the time-scaled set $\frac{1}{2t}\Upsilon$; this is one of the variants of what some authors refer to as *Dollard's theorem*.

As $\psi = \Omega_+\psi_+$, we can rewrite it in in the following way:

$$\psi = \Omega_+\psi_+ = \Omega_-\Omega_-^{-1}\Omega_+\psi_+ = \Omega_- S^{-1}\psi_+, \tag{97}$$

where $S : L^2(\mathbb{R}^m) \longrightarrow L^2(\mathbb{R}^m)$ with $S \coloneqq \Omega_+^{-1}\Omega_-$ is the *scattering operator*, often found in the physics literature as the *S-matrix*[89]. Thus, equation (97) implies via the definition of Ω_- and the isometricity of e^{-itH} that

$$\lim_{t\to-\infty} \|e^{-itH}\psi - e^{-itH_0}S^{-1}\psi_+\| = 0,$$

which is an invitation to apply Lemma D.3 once again:

$$\begin{aligned}
\sigma_\psi^{\mathrm{OQM}}(\Xi) &= \lim_{t\to-\infty} \int_{C(\Xi)} \left|(e^{-itH}\psi)(\mathbf{x})\right|^2 d^m x \\
&= \lim_{t\to-\infty} \int_{C(\Xi)} \left|(e^{-itH_0}S^{-1}\psi_+)(\mathbf{x})\right|^2 d^m x \\
&= \int_{-C(\Xi)} \left|(\mathcal{F}S^{-1}\psi_+)(\mathbf{k})\right|^2 d^m k,
\end{aligned} \tag{98}$$

[86] We will reserve $\mathbf{x}$ and $\mathbf{k}$ for the configuration space variable of the elements of $\mathfrak{D}(\mathcal{F})$ and $\mathfrak{R}(\mathcal{F})$, respectively, such that the reader will connect them easier with their physical meaning: see the next paragraph.

[87] Remember that we set $m = 1/2$.

[88] Owing as well to the fact that $\mathcal{F}$ is isometric, so $\|\mathcal{F}\psi\| = \|\psi\| = 1$.

[89] S^{-1} exists as the codomains of $\Omega_\pm$ agree, so we have $S\mathfrak{D}(\Omega_-) = \Omega_+^{-1}\Omega_-\mathfrak{D}(\Omega_-) = \Omega_+^{-1}\mathfrak{R}(\Omega) = L^2(\mathbb{R}^m) = \cdots = S^{-1}\mathfrak{D}(\Omega_+)$. Although it would have been more natural for our treatment to have '$S \coloneqq \Omega_-^{-1}\Omega_+$', as the scattering operator is here just a device to expose Ω_-, we chose to stick to the original physics notation. Nevertheless, S will appear in the analogous formula, when we will take $\psi = \Omega_-\psi_-$.

where (96) has been used for the last identity. The result (98) is important enough to recast it as:

Theorem 2.4 (Dollard's scattering-into-cones theorem)**.** *For $V \in L^1(\mathbb{R}^m) \cap L^2(\mathbb{R}^m)$ and an arbitrary state $\psi \in \mathfrak{R}(\Omega)$, and with $\psi_+,\ \psi_- \in L^2(\mathbb{R}^m)$ such that $\psi = \Omega_+\psi_+ = \Omega_-\psi_-$, the quantities*

$$\int_{-C(\Xi)} |(\mathcal{F}S^{-1}\psi_+)(\mathbf{k})|^2 \, d^m k \tag{99}$$

and

$$\int_{C(\Xi)} |(\mathcal{F}S\psi_-)(\mathbf{k})|^2 \, d^m k \tag{100}$$

are equal, both being alternate formulae for the scattering cross section

$$\sigma_\psi^{OQM}(\Xi) = \lim_{t\to\pm\infty} \int_{C(\Xi)} |(e^{-itH}\psi)(\mathbf{x})|^2 \, d^m x.$$

The theorem above is memorable as it indeed connects, via S and S^{-1}, the large t behaviour of an initial state $\psi \in \mathfrak{R}(\Omega)$ scattered by a potential $V \in L^1(\mathbb{R}^m) \cap L^2(\mathbb{R}^m)$ and with the IAS ψ_+ and OAS ψ_-, thus strengthening our belief that $\Omega_\pm$ should be a central part of scattering theory, at least for *short-range potentials*.

But shouldn't we be bothered that $\Omega_\pm$ might not exist for *long-range potentials*[90], and then the above analysis is not valid? Of course not, as firstly it would be unphysical to expect a particle scattered by a **long**-range potential to behave freely after a large period of time, as is the case for a **short**-range potential evolution. John D. Dollard fixed this mathematical issue with a solution that, quite surprisingly, extends the versatility of our approach to $\sigma_\psi^{\mathrm{OQM}}$ to Coulomb potentials; firstly, he observed that

$$\lim_{t\to-\infty} \|e^{-2itH} e^{itH_0}\psi_+ - e^{-itH}\Omega_+\psi_+\| = 0,$$

by the isometricity of e^{-itH} and the $t \to -\infty$ definition of the strong limit in Ω_+, i.e. $\text{s-lim}_{t\to-\infty} e^{-itH} e^{+itH_0} = \Omega_+$. A similar result can be proven also for $\psi = \Omega_-\psi_-$ in the limit $t \to +\infty$, hence Lemma D.3 paves the way to find yet another two formulae for $\sigma_\psi^{\mathrm{OQM}}$, i.e.

$$\begin{aligned} &\lim_{t\to-\infty} \int_{C(\Xi)} \left|(e^{-2itH} e^{itH_0}\psi_+)(\mathbf{x})\right|^2 \, d^m x, \\ &\lim_{t\to+\infty} \int_{C(\Xi)} \left|(e^{-2itH} e^{itH_0}\psi_-)(\mathbf{x})\right|^2 \, d^m x, \end{aligned} \tag{101}$$

which are in their own right interesting, as they serve the same conceptual purpose as (99) and (100), i.e. rewriting $\sigma_\psi^{\mathrm{OQM}}$ via the connection between an initial state ψ and its

[90] In [Teu99], a short-range potential is defined as one for which $V(\mathbf{x}) = O(|\mathbf{x}|^{-1-\varepsilon})$ for $|\mathbf{x}| \to \infty$ and an $\varepsilon > 0$, while a long-range potential is one for which the short-range condition does not apply.

corresponding IOAS $\psi_\pm$; the perk here is that we have gotten rid of $\Omega_\pm$, so will (101) hold also in the case $\mathfrak{D}(\Omega_\pm) = \{0_{L^2}\}$? We derived them using physically realistic $\psi_\pm \neq 0_{L^2}$, so of course not! But John D. Dollard drew a lot of inspiration from (101): he tried to find 'non-free' IOAS in the case of the Coulomb potential, i.e. functions that play the same role for the scattering via a Coulomb potential as $\psi_\pm$ does for a short-range potential. In this specific context, he defined $\Omega_\pm$-like operators, and with the 'non-free' IOAS, he proved results that mimic the formulae (99), (100), (101). The exact details can be found in [Dol64].

3. An introduction to Bohmian mechanics, with a focus on scattering theory

In Subsection 3.1-3.4 we will concisely present the basics of Bohmian mechanics (BM), the interpretation of QM introduced by David Bohm [Boh52] using earlier insights due to Louis de Broglie [Bro27]. Later on, in Subsection 3.5, we will argue that BM provides us with a clear understanding regarding the nature of scattering: as such, in Section 4, we will use BM to present a new take on the mathematics of scattering, albeit restricted to a single particle.

The present section is based heavily on the great reference [DT09], with further background details extracted from [Teu99], [DGZ92], and [DGZ96].

3.1. The seed of a new quantum theory

The so-called *weak measurements*[91] allow us to determine the average trajectories of photons passing through a two-slit interferometer, as it can be seen in Figure 5.

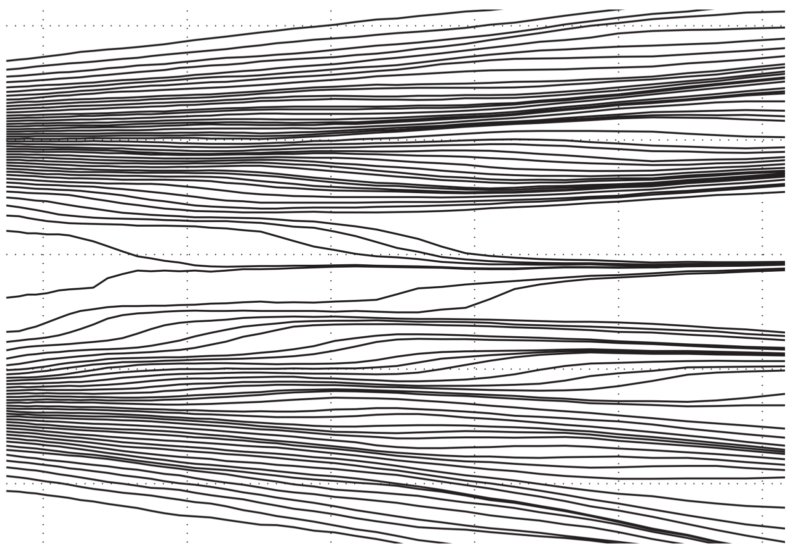

Figure 5: Photons passing through a two-slit interferometer (the slits are on the left). Notice that the perpendicular to the separation between the two slits seems to be an axis of symmetry. From [KBR$^+$11].

The question follows: can we really assign definite positions for the particles, and then determine their trajectories? On one hand, we have that the tried and true Heisenberg's

[91] Introduced for the first time under this name in [AAV88]. See [ACE14] for a discussion about weak measurements that includes counterarguments to their main points of criticism.

uncertainty principle forbids 'sharp' trajectories, while on the other hand Figure 5 is as convincing as possible. Is it possible to construct a coherent theory that reconciles the two contradictory, yet experimentally confirmed paradigms? Of course this is not[92] possible: as we will see in the remainder of this section, the contradiction is only apparent.

3.2. Symmetry and Bohmian mechanics

Suppose one has a particle with its position[93] represented by the Cartesian coordinates $(x, y, z) =: \mathbf{x} \in \mathbb{R}^3$, and with mass m. We are interested in the dynamics of its positions, i.e. to find how the vector

$$\mathbf{x}(t) = (x(t), y(t), z(t)) \tag{102}$$

changes with time. How shall we proceed? More precisely, can one expect to derive from scratch an equation that entails the time evolution of (102)? Are there any meaningful experiments that can aid us in the feat that lies ahead of us? Well, in view of what has been discussed in Subsection 1.1 and Subsection 1.2, we expect that some quantities of interest to be restricted to anything but an interval of the real axis. But this is meager for the context at hand, and even makes us stray from the essential feature of our particle: that it lives in the 3D Euclidean space! From pure reasoning about the Nature, we expect the equations of motion that describe our theory to be invariant under certain transformations of the underlying space. In the case of the 3D Euclidean space, its transformations are well-understood and give rise to *symmetries*, and the common sense thus corroborates that any of its physical laws should obey them, i.e. be invariant under *space translations*, *rotations about the origin*, and *Galilean boosts*. Moreover, if one has the time axis in mind, it comes naturally that the physical law that we seek to describe the time evolution of (102) should be invariant under *time shifts* and *time reversal*.

But first let us make things more precise. It may well happen[94] that the transformations we mentioned are representations $[g]$ of the elements g of a group G. As $\mathbf{x}(t) \in \mathbb{R}^3$, we

[92]Otherwise we would have that 'Nature is wrong.'!

[93]We start our derivation of BM with a fresh perspective towards the Nature as a whole, ignoring any insights that come from OQM, like e.g. the impossibility of attaching a definite position to particles, as prescribed by Heisenberg's uncertainty principle. Nevertheless, as it is essential that any theory, in particular BM, agrees with experimental facts, we will explain how one can recover Heisenberg's uncertainty principle at a latter stage (in Subsection 3.4).

[94]This is the case of e.g. the rotations around the origin of the Cartesian coordinate system we endowed $\mathbb{R}^3$ with; the relevant group $SO(3)$, which we will specify explicitly in a moment, is a subgroup of $GL_3(\mathbb{R})$, the group formed by the 3×3 invertible matrices equipped with the operation of standard matrix multiplication.

thus have that $[g] \in \mathbb{R}^{3\times 3}$, for which we introduce the notation

$$(g\mathbf{x})(t) \coloneqq [g]\mathbf{x}(t).$$

Consequently, if $\mathbf{x}(t)$ is in the solution set $\mathfrak{S}$ of an equation describing our physical law, we say that the latter obeys the symmetry implied by the group G if and only if the orbit of the group is in $\mathfrak{S}$ as well, by which we mean

$$G \cdot \mathbf{x}(t) \coloneqq \{(g\mathbf{x})(t) : g \in G\} \subseteq \mathfrak{S}.$$

More generally, if a transformation of $\mathbf{x}(t) \in \mathfrak{S}$ is encoded by an operator A, we say that the equation describing the physical law obeys the symmetry if

$$\widetilde{\mathbf{x}}(t) \coloneqq A\mathbf{x}(t) \in \mathfrak{S}.$$

Back to our particle. If we are interested in the time evolution of $\mathbf{x}(t)$, then a natural approach is to find an explicit expression for a vector field $\mathbf{v}(\mathbf{x}(t), t) \in \mathbb{R}^3$ such that

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{v}(\mathbf{x}(t), t). \tag{103}$$

In view of (103), we are looking for a *first order theory*, i.e. a theory in which the primal variable $\mathbf{x}(t)$ appears as the first order derivative with respect to t. As our particle lives in $\mathbb{R}^3$, perhaps the first symmetry that should come to our mind is the most tricky one: the symmetry under rotations about the origin, encoded in the elements of the set $SO(3) \coloneqq \{R \in GL_3(\mathbb{R}) : \det(R) = 1 \text{ and } R^T R = I\}$, which turns out to be a group on its own. Hence symmetry under $SO(3)$, i.e. the fact that we impose

$$\frac{d\widetilde{\mathbf{x}}(t)}{dt} = \mathbf{v}(\widetilde{\mathbf{x}}(t), t)$$

for $\widetilde{\mathbf{x}}(t) \coloneqq R\mathbf{x}(t)$, $\forall R \in SO(3)$, can be implemented as follows: using an insightful[95] comparison with the equation from Hamiltonian mechanics

$$\mathbf{v}(\mathbf{x}(t), t) = \frac{1}{m}\nabla S(\mathbf{x}(t), t), \tag{104}$$

which tells us that the **classical** velocity vector field $\mathbf{v}$ is generated by taking the gradient of a scalar function[96] S, we have by analogy that it might be useful to find a complex-valued ψ such that

$$\mathbf{v}(\mathbf{x}(t), t) \sim \nabla\psi(\mathbf{x}(t), t). \tag{105}$$

[95] At this step more in a mathematical, rather than in a physical way, as we try to derive a theory that is able to accommodate nonclassical behaviour. Nevertheless, the Hamilton-Jacobi equation of CM from which (104) was derived poses some very interesting properties [DT09, p.24-p.26], as it was created in analogy with wave optics, and we are prone to think that waves are intimately connected to the quantum world owing to the wave-particle duality.

[96] Nothing else but the action. Its gradient transforms 'like a vector', as one can readily verify.

Now, Sir William Rowan Hamilton came with the eponymous formulation of CM that leads to (104) by thinking of S as a wave that guides the **classical** trajectory $\mathbf{x}(t)$ of a particle with mass m, having in the back of his mind Huygens' principle. Similarly, it is not presumptuous to think that $\psi(\mathbf{x}(t), t)$ will turn out to be a wave as well. To see how a wave should behave under transformations that give rise to symmetries, let us take a simple case: the general equation of a plane wave is

$$\psi(\mathbf{x}(t), t) = \mathcal{A}e^{i(\mathbf{k}\cdot\mathbf{x}(t)-\omega t)}, \tag{106}$$

where $\mathbf{k} \in \mathbb{R}^3$, and ω, $\mathcal{A} \in \mathbb{R}^+$.

Subsequently, suppose that we search for an operator T_{rev} that maps $\mathbf{x}(t)$ to its time reversed version $\widetilde{\mathbf{x}}(t)$. We should be very careful about this: although T_{rev} is naturally the mapping that replaces t with $-t$, in the sense that $T_{\text{rev}}\mathbf{x}(t) = \mathbf{x}(-t)$, $\psi_{\text{rev}}(\mathbf{x}(t), t)$ should be a wave that preserves some of the features of the initial wave, i.e. the wave $\psi(\mathbf{x}(t), t)$ before we reverted[97] the time. Should then the initial wave simply transform under time inversion as

$$\psi(\mathbf{x}(t), t) \to \psi(\mathbf{x}(-t), -t) \ ?$$

Well, a quick glance at (106) tells us that if we just flip the sign of t, then this will imply that the 'naively' reversed wave has an identical phase[98], and not a time reversed one, which is an undesirable feature. Considering this, we expect that the initial wave should be time reversed according to

$$\psi(\mathbf{x}(t), t) \to \psi^*(\mathbf{x}(-t), -t), \tag{107}$$

which takes care that the phase is time reversed, while still preserving the common sense 'reversion of a reversed wave' $\psi^*(\mathbf{x}(-t), -t) \to \psi(\mathbf{x}(t), t)$.

Also common sense determines us to find an equation for our physical law that is symmetric under time reversal, i.e. for which it is true that:

$$\mathbf{x}(t) \text{ a solution, for wave } \psi(\mathbf{x}(t), t) \iff \mathbf{x}(-t) \text{ a solution, for wave } \psi^*(\mathbf{x}(-t), -t).$$

We then find useful to recast (105) together with (103) as

$$\frac{d\mathbf{x}(t)}{dt} \sim \nabla\psi(\mathbf{x}(t), t). \tag{108}$$

[97]By which we simply mean that for $t_1 < t_2$, t_1 is the latter time; equivalently, we invert the arrow of time.

[98]Prosaically said, the ω in the $e^{-i\omega t}$ part of the initial wave plays the same role as the ω in the $e^{i\omega t}$ part of the 'naively' time reversed wave (as we now index our events according to $-t$), so that the initial wave and the 'naively' time reversed one travel in the same direction, which is nonsense.

Notice that the left-hand side of (108) picks a minus sign if we first transform $T_{\text{rev}}\mathbf{x}(t) = \mathbf{x}(-t)$ and then differentiate it, while on the right-hand side we need to use[99] (107). To mirror the minus obtained on the left-hand side, and also to get rid of the inconvenient fact that we have on the left-hand side a real quantity, while on the right-hand side there is a complex one, we take the imaginary part of the right-hand side to obtain

$$\frac{d\mathbf{x}(t)}{dt} \sim \operatorname{Im}\{\nabla\psi(\mathbf{x}(t),t)\}, \tag{109}$$

or, by using the vector field $\mathbf{v}(\mathbf{x}(t),t)$,

$$\mathbf{v}(\mathbf{x}(t),t) \sim \operatorname{Im}\{\nabla\psi(\mathbf{x}(t),t)\}. \tag{110}$$

Further, we point that for *space translations*

$$T_{\mathbf{a}}\mathbf{x}(t) \coloneqq \mathbf{x}(t) + \mathbf{a},$$

with $\widetilde{\mathbf{x}}(t) \coloneqq T_{\mathbf{a}}\mathbf{x}(t)$, we have that

$$\frac{d\widetilde{\mathbf{x}}(t)}{dt} = \frac{d\mathbf{x}(t)}{dt},$$

and that

$$\operatorname{Im}\{\nabla\psi(\mathbf{x}(t),t)\} = \operatorname{Im}\{\widetilde{\nabla}\psi(\widetilde{\mathbf{x}}(t),t)\},$$

both following from straightforward calculations. Hence, it seems that if our equation is being derived with the specification (109), it turns out to be automatically symmetric under space translations. Similarly, showing that (109) is already symmetric under *time shifts*, encoded in the operator T_s that satisfies $T_s\mathbf{x}(t) = \mathbf{x}(t+s)$ for a constant $s \in \mathbb{R}$, is trivial.

Therefore, let us turn our attention to the more interesting *Galilean boosts*, i.e. transformations[100] of the type

$$B_{\mathbf{u}}\mathbf{x}(t) \coloneqq \mathbf{x}(t) + \mathbf{u}t,$$

with $\mathbf{u}$ representing the constant velocity of another frame of reference with respect to the frame of reference where $\mathbf{x}(t)$ lies. By replacing $\mathbf{x}(t)$ with $\widetilde{\mathbf{x}}(t) \coloneqq B_{\mathbf{u}}\mathbf{x}(t)$ in (109), we obtain that the right-hand side should obey

$$\operatorname{Im}\nabla\{\psi(\mathbf{x}(t),t)\} + \mathbf{u} = \operatorname{Im}\{\widetilde{\nabla}\psi(\widetilde{\mathbf{x}}(t),t)\}. \tag{111}$$

[99] The gradient is acting over the spatial coordinates, hence no minus sign appears on the right-hand side of (108) if we replace $\psi(\mathbf{x}(t),t)$ with $\psi^*(\mathbf{x}(-t),-t)$.

[100] Although the Galilean boosts, along with translations, can be efficiently represented by matrices that are representations of a subset of the Galilean group, we will not introduce them explicitly (but see [FM06, p.71]).

Basically, we are looking for a relation between $\psi(\mathbf{x}(t),t)$ and $\psi(\widetilde{\mathbf{x}}(t),t)$ that implies (111), i.e. we want to describe explicitly the transformation $\psi(\mathbf{x}(t),t) \to \psi(\widetilde{\mathbf{x}}(t),t)$. By reasonably setting

$$\psi(\widetilde{\mathbf{x}}(t),t) \coloneqq e^{i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha}\psi(\mathbf{x}(t),t), \tag{112}$$

where α is just a constant that takes care that the combination $\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha$ is dimensionless, we see that

$$\begin{aligned}
\mathrm{Im}\{\widetilde{\nabla}\psi(\widetilde{\mathbf{x}}(t),t)\} &= \mathrm{Im}\left\{\widetilde{\nabla}(e^{i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha}\psi(\mathbf{x}(t),t))\right\} \\
&= \mathrm{Im}\left\{(\widetilde{\nabla}e^{i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha})\psi(\mathbf{x}(t),t) + e^{i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha}(\widetilde{\nabla}\psi(\mathbf{x}(t),t))\right\} \\
&= \mathrm{Im}\left\{((i\mathbf{u}/\alpha)e^{i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha})\psi(\mathbf{x}(t),t) + e^{i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha}(\nabla\psi(\mathbf{x}(t),t))\right\} \\
&= \mathrm{Im}\left\{(i\mathbf{u}/\alpha)\psi(\widetilde{\mathbf{x}}(t),t) + e^{i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha}(\nabla\psi(\mathbf{x}(t),t))\right\},
\end{aligned} \tag{113}$$

which is definitely reminiscent of (111); what is missing, though? On the last line of (113) we have an extra factor $\psi(\widetilde{\mathbf{x}}(t),t)$ that impedes us to pull $\mathbf{u}/\alpha$ out of the $\mathrm{Im}\{\dots\}$, while the other term is multiplied with an undesirable factor $e^{i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha}$. This can be fixed most easily if we would impose instead that

$$\frac{d\mathbf{x}(t)}{dt} \sim \mathrm{Im}\left\{\frac{\nabla\psi(\mathbf{x}(t),t)}{\psi(\mathbf{x}(t),t)}\right\},$$

turning the invariance condition into

$$\mathrm{Im}\left\{\frac{\nabla\psi(\mathbf{x}(t),t)}{\psi(\mathbf{x}(t),t)}\right\} + \mathbf{u} = \mathrm{Im}\left\{\frac{\widetilde{\nabla}\psi(\widetilde{\mathbf{x}}(t),t)}{\psi(\widetilde{\mathbf{x}}(t),t)}\right\},$$

as then

$$\begin{aligned}
\alpha\mathrm{Im}\left\{\frac{\widetilde{\nabla}\psi(\widetilde{\mathbf{x}}(t),t)}{\psi(\widetilde{\mathbf{x}}(t),t)}\right\} &= \alpha\mathrm{Im}\left\{\frac{\widetilde{\nabla}(e^{i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha}\psi(\mathbf{x}(t),t))}{\psi(\widetilde{\mathbf{x}}(t),t)}\right\} \\
&= \alpha\mathrm{Im}\left\{\frac{(i\mathbf{u}/\alpha)\psi(\widetilde{\mathbf{x}}(t),t)}{\psi(\widetilde{\mathbf{x}}(t),t)} + \frac{e^{i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/\alpha}(\nabla\psi(\mathbf{x}(t),t))}{\psi(\widetilde{\mathbf{x}}(t),t)}\right\} \\
&= \alpha\mathrm{Im}\left\{i\frac{\mathbf{u}}{\alpha} + \frac{\nabla\psi(\mathbf{x}(t),t)}{\psi(\mathbf{x}(t),t)}\right\} \\
&= \mathbf{u} + \alpha\mathrm{Im}\left\{\frac{\nabla\psi(\mathbf{x}(t),t)}{\psi(\mathbf{x}(t),t)}\right\},
\end{aligned} \tag{114}$$

which has the same physical value as (111), as α is just a constant.

As we ran dry of symmetries to impose, we can conclude that

$$\frac{d\mathbf{x}(t)}{dt} = \alpha\mathrm{Im}\left\{\frac{\nabla\psi(\mathbf{x}(t),t)}{\psi(\mathbf{x}(t),t)}\right\}, \tag{115}$$

for a suitably chosen α specified by (112).

To recapitulate, we started with the assumption that we need to find a vector field $\mathbf{v}$ that generates the time evolution of a particle of mass m, in the sense of (103). We just found that if the aforementioned vector field is of the form

$$\mathbf{v}^{\psi}(\mathbf{x}(t),t) \coloneqq \alpha \mathrm{Im}\left\{\frac{\nabla\psi(\mathbf{x}(t),t)}{\psi(\mathbf{x}(t),t)}\right\}, \tag{116}$$

then the equation we derive is, in the order we proceeded, invariant under rotations about the origin, time reversal, space translations, time shifts, and Galilean boosts.

As can be seen in (116), we changed for once the notation such that it is clear that the vector field is dependent on ψ. Thus it is the right time to turn our attention to the latter: we need to find an equation for ψ that obeys the same symmetries as before. We can count out time reversal for a moment and propose Poisson's equation

$$\text{‘}\nabla^2\psi(\mathbf{x}(t),t) = f(\mathbf{x}(t))\text{’} \tag{117}$$

as the simplest equation that obeys the other symmetries, as it can be shown using a similar approach as before. However, we expect ψ to be a wave! Consequently, the fact that under time reversal we have the unusual $\psi(\mathbf{x}(t),t) \to \psi^*(\mathbf{x}(-t),-t)$, i.e. that ψ should be conjugated when we reverse time, motivates us to extend (117) to an equation where ψ will be assumed to change with time. The next simplest equation for ψ with these features is

$$i\frac{\partial\psi(\mathbf{x}(t),t)}{\partial t} = \beta\nabla^2\psi(\mathbf{x}(t),t), \tag{118}$$

where the imaginary number i has been added to satisfy symmetry under time reversal, and β is a general constant coming from the Nature itself, to be determined at a latter stage.

However, up until now we completely ignored the fact that the dynamics of our particle can be influenced by the intrinsic physical properties of the space where it resides, a situation we are well familiar[101] with. Thus, we minimally extend (118) by adding to its right-hand side the quantity $F(\mathbf{x}(t))\psi(\mathbf{x}(t),t)$, with F real-valued given by the physical properties of the space where our particle is located, so that we now have

$$i\frac{\partial\psi(\mathbf{x}(t),t)}{\partial t} = \beta\nabla^2\psi(\mathbf{x}(t),t) + F(\mathbf{x}(t))\psi(\mathbf{x}(t),t), \tag{119}$$

an equation[102] that obeys all the symmetries we discussed above, as can be easily checked.

[101] E.g. the motion of any point object on Earth is influenced by the gravitational potential, a situation that comes as an extra from the fact that it lives in $\mathbb{R}^3$.

[102] Perhaps the reader might see the ‘shape’ of the time-dependent Schrödinger equation profiling in (119). At the end of the next subsection, once we determined β, we will indeed confirm that this is the case.

In the next subsection, we will firstly find the link between α and β, and then finally determine[103] α, as only then we can use (115) and (119) to provide a full description of the position[104] $\mathbf{x}(t)$ of our particle.

3.3. The dynamics of a Bohmian system

In the previous subsection we claimed that (119) is, among other things, invariant under Galilean boosts. The connection between α as in (115) and β as in (119) surfaces easily if we explicitly specify the transformation $\psi(\mathbf{x}(t), t) \to \psi(\widetilde{\mathbf{x}}(t), t)$, in an identical spirit to (112). In view of this, the transformation is

$$\psi(\widetilde{\mathbf{x}}(t), t) := e^{-i\widetilde{\mathbf{x}}(t)\cdot\mathbf{u}/2\beta}\psi(\mathbf{x}(t), t),$$

which implies that $\alpha = -2\beta$.

Although connecting α with β was done with respect to symmetry arguments, and therefore the reader may wonder why we have not included the above argument in the previous subsection, it is nevertheless useful to see clearly that we are now left only with determining α: no symmetries are left, and even if they were, that would certainly not be the way to proceed, as they can only provide us with insights regarding the 'shape' of the equation(s) of the sought physical law.

Thus, let us rewrite the complex-valued ψ in the following way

$$\psi(\mathbf{x}(t), t) = U(\mathbf{x}(t), t)e^{iM(\mathbf{x}(t),t)/\gamma}, \tag{120}$$

where $\mathbf{x}(t) \in \mathbb{R}^3$, U and M are real-valued, and γ is just a constant[105] that takes care that the combination $M(\mathbf{x}(t), t)/\gamma$ is dimensionless. Substituting (120) in (115), we obtain

$$\frac{d\mathbf{x}(t)}{dt} = \frac{\alpha}{\gamma}\nabla M(\mathbf{x}(t), t) \tag{121}$$

which can be efficiently compared with (104), recasted as

$$\frac{d\mathbf{x}(t)}{dt} = \frac{1}{m}\nabla S(\mathbf{x}(t), t),$$

in the sense that the vector field on the left-hand side of both equations is generated by the gradient of M and S, respectively. From the point of view of units, this suggests that we should simply identify $\alpha \equiv \gamma/m$; we will double-check this at a later stage.

[103] As the mass m did not appear yet anywhere, we expect that α will include it.

[104] However, before the excitement of such a perspective overcomes us, it is worth mentioning that determining $\mathbf{x}(t)$ explicitly turns out not to be very enlightening in many cases (see [Tes14, p.153-p.158]); instead, the strength of BM is to provide valuable new conceptual insights where OQM is too vague, as is the case of scattering theory. We will turn to this aspect in Subsections 3.4-3.5.

[105] Although it seems like our reasoning is circular, in the sense that now we will have to find a relation between α and γ, and then determine α, hang on for a bit!

Now, let us finally find 'who' is γ: we fortunately have one more equation to feed (120), namely (119). By doing this we encounter some pesky calculations, which we will skip here (but see [DT09, p.149]); however, by taking the real and the imaginary part of the ensuing equation, respectively, and by rearranging with respect to (121), we get

$$\frac{\partial U^2(\mathbf{x}(t),t)}{\partial t} = -\nabla \cdot \left(\frac{d\mathbf{x}(t)}{dt}U^2(\mathbf{x}(t),t)\right), \tag{122}$$

for the imaginary part, which does not ring a bell at this stage, but for the real part we have

$$\frac{\partial M(\mathbf{x}(t),t)}{\partial t} + \frac{\alpha}{2\gamma}(\nabla M(\mathbf{x}(t),t))^2 + \gamma F(\mathbf{x}(t)) - \frac{\alpha\gamma}{2}\frac{\nabla U(\mathbf{x}(t),t)}{U(\mathbf{x}(t),t)} = 0, \tag{123}$$

which is qualitatively **almost** the same as the Hamilton-Jacobi differential equation in the case of a Newtonian particle of mass m:

$$\frac{\partial S(\mathbf{x}(t),t)}{\partial t} + \frac{1}{2m}(\nabla S(\mathbf{x}(t),t))^2 + V(\mathbf{x}(t)) = 0. \tag{124}$$

Comparing the second term in (123) with the second one in (124), we strengthen our belief that the identification $\alpha \equiv \gamma/m$ was justified. Now we can move to the third term: we wonder whether we can ignore the fourth term in (123), and simply infer that the third terms of (123) and (124) represent the same thing. Yes, we can do this, as we remind the reader that F in (123) comes as an adjustment to the physical properties of the space the particle lives in, and we know from CM that this is exactly the role of the potential V in (124). So, by identifying $V \equiv \gamma F$, we can see that the fourth term, which we will call the *quantum potential*, is a deviation from CM, as encoded in (124); thus the condition

$$\left|\frac{\alpha\gamma}{2}\frac{\nabla U(\mathbf{x}(t),t)}{U(\mathbf{x}(t),t)}\right| \ll |V(\mathbf{x}(t))| \tag{125}$$

ensures that the Bohmian trajectory degenerates to the classical one.

Surprisingly enough, γ can be determined from a specific wave that renders the quantum potential null. Suppose that the wave is $\psi_{\mathrm{dB}}(\mathbf{x}(t),\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}(t)}$, such that $M(\mathbf{x}(t),t) = \gamma\mathbf{k}\cdot\mathbf{x}(t)$ and $U(\mathbf{x}(t),t) = 1$. Then for short periods of time, for which $\mathbf{x}(t)$ is not changing much, we can interpret (121) as being the classical velocity of the particle[106], i.e.

$$\mathbf{v}_{\mathrm{cl}}^{\psi_{\mathrm{dB}}}(\mathbf{x}(t),t) \equiv \frac{d\mathbf{x}(t)}{dt} = \frac{\gamma\mathbf{k}}{m},$$

[106] Partly by what we mentioned before, that if (125) is true, the particles will follow classical trajectories. However, this assertion necessitates a complete discussion on the topic of the classical limit of BM, to be found in [DT09, p.186-191].

and, via the de Broglie hypothesis which tells us that $\psi_{\mathrm{dB}}(\mathbf{x}(t), \mathbf{k})$ has momentum

$$\mathbf{p} = \hbar\mathbf{k},$$

we can then identify $\gamma \equiv \hbar$.

Finally, the observation that now $\beta = -\gamma/2m = -\hbar/2m$, and by $V \equiv \gamma F = \hbar F$, we are prompted to identify (119) as the one-particle Schrödinger equation, which is, in a way, a relief, although we stress that now (119) does not belong to OQM, but to BM, as will be explained in the next two subsections.

Let us recast the equations generating the Bohmian dynamics of a particle in their final form:

$$\frac{d\mathbf{x}(t)}{dt} = \frac{\hbar}{m}\mathrm{Im}\left\{\frac{\nabla\psi(\mathbf{x}(t), t)}{\psi(\mathbf{x}(t), t)}\right\} \tag{126}$$

prescribes the Bohmian trajectory of a particle with mass m under the influence of a potential V that is enclosed in ψ obtained from solving

$$i\frac{\partial\psi(\mathbf{x}(t), t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}(t), t) + V(\mathbf{x}(t))\psi(\mathbf{x}(t), t). \tag{127}$$

The generalization[107] to an N-particle system is straightforward:

$$\frac{d\mathbf{X}(t)}{dt} = \hbar M^{-1}\mathrm{Im}\left\{\frac{\nabla\psi(\mathbf{X}(t), t)}{\psi(\mathbf{X}(t), t)}\right\}, \tag{128}$$

and

$$i\frac{\partial\psi(\mathbf{X}(t), t)}{\partial t} = -\frac{\hbar^2}{2}M^{-1}\nabla^2\psi(\mathbf{X}(t), t) + V(\mathbf{X}(t))\psi(\mathbf{X}(t), t), \tag{129}$$

where $\mathbf{X}(t) := (\mathbf{x}_1(t), \ldots, \mathbf{x}_N(t))$ is their common position in the configuration space $\mathbb{R}^{3N}$, and $M := (\delta_{ij}m_j) \in \mathbb{R}^{3N} \times \mathbb{R}^{3N}$ is the mass matrix. The Bohmian trajectory for the i-th particle is obtained by first solving the N-particle Schrödinger equation (129), and then

$$\frac{d\mathbf{x}_i(t)}{dt} = \frac{\hbar}{m_i}\mathrm{Im}\left\{\frac{\nabla_i\psi(\mathbf{X}(t), t)}{\psi(\mathbf{X}(t), t)}\right\},$$

for $i = 1, \ldots, N$.

And if we use (128) and (129) to simulate particles that are passing through a two-slit interferometer, we obtain:

---

[107] Needless to say, although we derived the equations that generate the Bohmian dynamics of a particle for $\mathbb{R}^3$, they are equally valid for $\mathbb{R}^m$ as well.

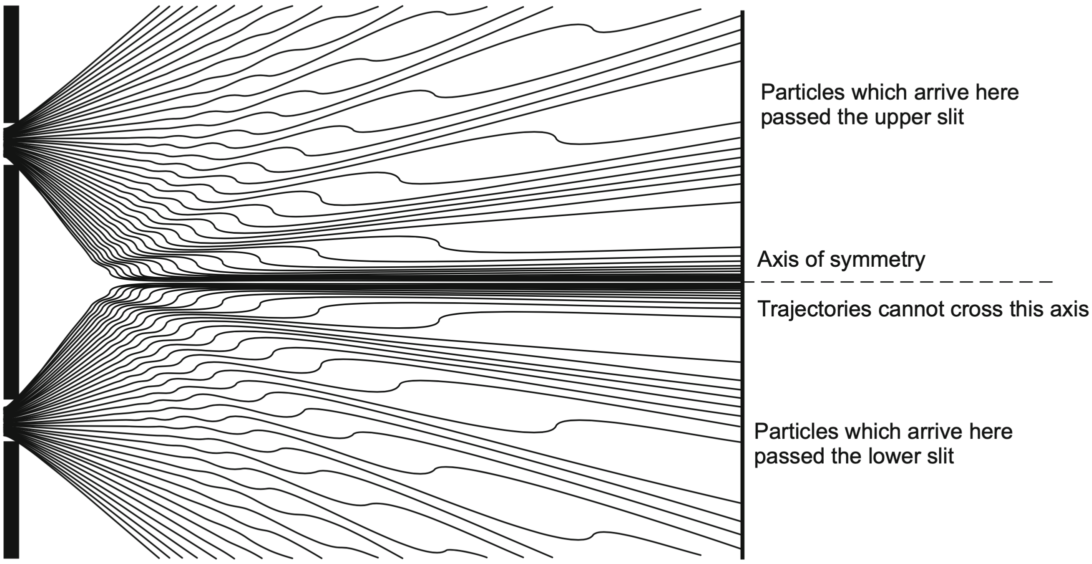

Figure 6: Simulated Bohmian trajectories of particles passing through a two-slit. From [DT09, p.156].

which is indeed qualitatively similar[108] to Figure 5.

3.4. The quantum equilibrium hypothesis and its implications

One might be justifiably worried that by adding the equation (126) to the standard[109] one-particle Schrödinger equation (127), we have derived a so-called 'hidden variable theory', in this case the hidden variable being the Bohmian position $\mathbf{x}(t)$. Indeed, everything looks very deterministic, in the sense that by **specifying** an initial position $\mathbf{x}(0)$ one can solve[110] (126) given ψ to obtain the Bohmian trajectory $\mathbf{x}(t)$ for all latter times. However, we know from experiments, not to say e.g. Heisenberg's uncertainty principle yet, that Nature is probabilistic, so we should better explain now how chance enters BM.

We stressed 'specifying' in the paragraph above, however this is not what David Bohm had in mind when proposing (126) and (127) for the dynamics of a nonclassical particle. In fact, he hypothesised that the initial position $\mathbf{x}(0)$ is actually **distributed**

[108] Although (128) and (129) do not apply to photons, as they are massless.

[109] We return to our convention that $\hbar = 1$, $m = 1/2$ such that $H_0 = -\nabla$, as now our focus is on understanding the qualitative properties of the equations that generate the dynamics of a one-particle Bohmian system (126) and (127).

[110] Despite the worrying zeros of the ψ that appears in the denominator of the right-hand side of (126), the existence and uniqueness of solutions of the equations of BM has been proven for a large class of potentials in [BDG$^+$95]; the latter is the analogue of what Corollary A.2.1 implies for OQM.

according to a pdf $\rho(\mathbf{x}(0), 0)$, such that the Bohmian positions at latter times $\mathbf{x}(t)$ are distributed according to $\rho(\mathbf{x}(t), t)$. But how can we find or choose sensibly $\rho(\mathbf{x}(t), t)$? The most straightforward approach is to compare the continuity equation for $\rho(\mathbf{x}(t), t)$ that is transported along the Bohmian flow of a particle with the Bohmian 'velocity' $\mathbf{v}(\mathbf{x}(t), t) \coloneqq d\mathbf{x}(t)/\,dt$ as in (126):

$$\frac{\partial \rho(\mathbf{x}(t), t)}{\partial t} + \nabla \cdot (\rho(\mathbf{x}(t), t)\mathbf{v}(\mathbf{x}(t), t)) = 0, \tag{130}$$

with the quantum continuity equation[111] obtained from (127):

$$\frac{\partial |\psi(\mathbf{x}(t), t)|^2}{\partial t} + \nabla \cdot \mathbf{j}(\mathbf{x}(t), t) = 0, \tag{131}$$

where

$$\mathbf{j}(\mathbf{x}(t), t) \coloneqq |\psi(\mathbf{x}(t), t)|^2 \mathbf{v}(\mathbf{x}(t), t) = 2\mathrm{Im}\{\psi^*(\mathbf{x}(t), t)\nabla\psi(\mathbf{x}(t), t)\}. \tag{132}$$

We will refer to the above $\mathbf{j}$ as the *quantum flux*. Thus, it comes naturally to set[112]

$$\rho(\mathbf{x}(t), t) \coloneqq |\psi(\mathbf{x}(t), t)|^2.$$

What has been presented above goes by the name of the *quantum equilibrium hypothesis (QEH)* in BM:

For a particle having the normalized wave function ψ, the empirical distribution of $\mathbf{x}(t)$ is given **approximately** by $|\psi(\mathbf{x}(t), t)|^2$.

We recall that if $\|\psi(\mathbf{x}(0), 0)\| = 1$, then $\|\psi(\mathbf{x}(t), t)\| = 1$ as well for any $t \in \mathbb{R}$, according to Corollary A.2.1. Moreover, we stressed above 'approximately' such that the reader will infer that for most practical purposes, $|\psi(\mathbf{x}(t), t)|^2$ is really the pdf of $\mathbf{x}(t)$. A rigorous treatment of the latter point can be found in [DGZ92, p.32-p.37], where in fact the QEH becomes a well-grounded law of large numbers.

Therefore, one can see that Born's rule is a **consequence** of BM, as encoded in (126) and (127). Thus, for the so-called 'position measurements', BM is in full harmony with OQM, i.e. for a particle in an initial state $\psi \equiv \psi(\mathbf{x}(0), 0)$

$$P^{\psi}_{\mathrm{BM}}(\mathbf{x}(t) \in \Upsilon) = \int_{\Upsilon} |\psi(\mathbf{x}(t), t)|^2 \, d^3x = P^{\psi}_{\mathrm{OQM}}(\mathbf{x}(t) \in \Upsilon), \tag{133}$$

for a Borel measurable $\Upsilon \subseteq \mathbb{R}^3$, so we can safely drop the superscripts in (133). However, as our particle is now having a position, we know that it travels with the wave packet, if there is only one, of course.

[111] See (122).

[112] Which turns out to be a unique choice as well, under physically plausible conditions [GS07].

It is worth mentioning that the QEH refers to dynamics given by *typical* initial positions $\mathbf{x}(0)$. What do we mean by typical, though? We can replace it with 'too many such that the others do not really count', but then we can ask ourselves which are **the other**, i.e. atypical initial positions? This asks for a precise explanation, as quantitative as possible. Therefore, for the time being, we will digress from BM, and talk a bit about Ludwig Boltzmann's view of chance in physics.

Suppose Boltzmann's loyal German Shepherd is sleeping at his feet, obediently waiting for his master's all-nighter to reach an end. While Boltzmann sits with his elbows and beard resting gently on his bureau and ponders about Nature, he is not even in the slightest concerned about the fact that, say, all the molecules of air surrounding his dog underneath might suddenly leave the space around his feet and thus cause his friend's asphyxiation. Why is he so certain that this won't happen, though? Well, because his life's work rests on the existence of *microstates*, which deem the very situation described above as (almost) impossible. If he would pick an initial time $t = 0$ and 'record' all the initial positions and momenta of the molecules in his study, the possibility that the aforementioned will evolve as the time passes in such a way that they will cause his dog to succumb is highly unlikely, i.e. this murderous microstate[113] is *atypical*, in the sense that it leads to a very improbable *macrostate*. In mathematical language, the natural measure of the Boltzmann-Gibbs ensemble [Wer13] assigns a very small 'volume' to the set of initial positions and momenta of all the molecules such that they will deviate eventually from thermal equilibrium and kill Boltzmann's dog. This solves the mystery of Boltzmann's apparent carelessness for his dog's safety.

Similarly, $|\psi(\mathbf{x}(t),t)|^2$ gives us the *typicality measure* for BM

$$P(\mathbf{x}(t) \in \Upsilon) = \int_{\Upsilon} |\psi(\mathbf{x}(t),t)|^2 \, d^3x \approx 0,$$

[113] The following analogy might be helpful: suppose we have a box full with a billion euro cents (although this is pure fantasy given the scientists' wages); consequenly, we shake it vigorously, we open the lid, take one coin at a time, place it in order on the table and record its relative position (i.e. the 1367th coin that we drew) and whether it was facing head or tail. What is the probability that we will have the following microstate: a sequence of exactly a billion heads? Probability theory tells us that any sequence of the sort, irrespective of the number of heads or tails it entails, is equally likely $(1/2^{10^6})$, so this is not very illuminating. Instead, we should ask ourselves: what is the probability that we have the macrostate consisting of a billion heads? It is exactly $1/2^{10^6}$, as only the microstate $(H_1, H_2, \ldots, H_{10^6})$ leads to a count of a billion heads. However, what can we say about the probability of the macrostate consisting of half a billion heads? Probability theory gives us a precise answer also in this case, but we don't need it here to know that the chances of counting half a billion heads are way higher than counting a billion ones. There are many ways of arranging a sequence of half a billion heads and half a billion tails, in other words we have a large number of microstates that lead to the macrostate of counting half a billion heads, and this dwarfs by comparison the probability of getting a count of a billion heads. Thus, $(H_1, H_2, \ldots, H_{10^6})$ is atypical.

where $\Upsilon = \{\mathbf{x}(0) \in \mathbb{R}^3 : \mathbf{x}(t) \text{ is } \mathbf{not} \text{ distributed according to QEH}\}$. More on the topic of typicality in BM can be found in [DT09, Ch.11].

But let us get back to more pressing issues, namely the reconciliation between Heisenberg's uncertainty principle and BM. We remind the reader that the primal variable of BM is the position $\mathbf{x}(t)$, which appears in the OQM derivation of the principle, so it seems that there are no obstacles in understanding what the the quantities $\{\Delta_t(x_i)\}_{i=1}^3$ refer to: they are simply the standard deviations of the pdf $|\psi(\mathbf{x}(t), t)|^2$, i.e. the squared elements of the diagonal of its covariance matrix! However, would it be sensible to say that $\{\Delta_t(p_j)\}_{j=1}^3$ are obtained from $(v_1(\mathbf{x}(t), t), v_2(\mathbf{x}(t), t), v_3(\mathbf{x}(t), t)) = \mathbf{v}(\mathbf{x}(t), t) := d\mathbf{x}(t)/\,dt$ as in (126) via

$$\langle v_j \rangle_{\psi(t)} := \int_{\mathbb{R}^3} v_j(\mathbf{x}(t), t) |\psi(\mathbf{x}(t), t)|^2 \, d^3x$$

$$\langle v_j^2 \rangle_{\psi(t)} := \int_{\mathbb{R}^3} v_j^2(\mathbf{x}(t), t) |\psi(\mathbf{x}(t), t)|^2 \, d^3x$$

such that

$$\Delta_{\psi(t)}(p_j) = m\sqrt{\langle v_j^2 \rangle_{\psi(t)} - \langle v_j \rangle_{\psi(t)}^2} \; ?$$

Well, contrary to the OQM status quo, where Axiom 2 tells us the connection between CM and OQM observables, we do not have any reason to believe that $\mathbf{v}(\mathbf{x}(t), t)$ is corresponding to the CM velocity. Instead, the classical limit of BM [DT09, p.186-p.191] tells us that the BM quantity with the same physical meaning as the CM velocity is instead

$$\mathbf{v}_\infty(\mathbf{x}(t), t) = \lim_{t \to \infty} \frac{\mathbf{x}(t)}{t},$$

where the limit above should be understood as the convergence in the $|\psi(\mathbf{x}(t), t)|^2$-related distribution for $\mathbf{x}(t)/t$, as expounded in [DT09, p.306]. Thus, the BM version of Heisenberg's uncertainty principle turns into

$$\Delta_{\psi(t)}(x_i)\Delta_{\psi(t)}(p_\infty^j) \geq \frac{\delta_{ij}}{2}, \tag{134}$$

where $(p_\infty^1, p_\infty^2, p_\infty^3) = \mathbf{p}_\infty := m\mathbf{v}_\infty$. It turns out that Heisenberg's uncertainty principle is a **consequence** of the QEH: a rigorous derivation of (134) can be found in [DT09, p.306-310].

Let us turn our attention to nonlocality in BM. Now, the takeaway of Subsection 1.7 was that Nature and NISA[114] go hand in hand, and BM is a theory about Nature, so then

[114] We remind the reader the following: 'ISA' stands for informational superluminal action between spacelike separated events, i.e. sending a signal faster than light, which violates the principle of causality of special relativity, as from some inertial frames the signal will appear as travelling back in time; on the other hand, 'NISA' is non-informational superluminal action between spacelike separated events, a phenomenon that every theory of Nature should incorporate according to Bell's theorem.

we know that NISA should be part of it as well. Actually, similarly to OQM, BM leads to the same violation of Bell's inequality (66), as it is presented in [DT09, p.205-p.207], so NISA is really a feature pertaining to BM as well, which strengthens our belief in its plausibility. Why not ISA, though? For this, see [DT09, p.208-p.209].

Next, as we deal with spinless particles in this work, the BM take on spin should not preoccupy us much (but see [DGZ96, p.17-20]). However, surprisingly enough, BM shines some light on the very nature of spin: the reader might find it worth glancing over Tim Maudlin's thought experiment presented in [DT09, p.165-p.166].

Lastly, we reiterate that Bohm's motivation for creating his own interpretation of QM was to 'solve' the measurement problem. However, this feat requires a more detailed understanding of specific topics of BM that are not so relevant for nonrelativistic spinless one-particle scattering, hence we redirect the reader to the concise article [Mau95].

To conclude, Born's rule and Heisenberg's uncertainty principle are consequences of the QEH, the rigorously justified gateway of chance for BM. Moreover, QEH implies that BM is in full harmony with OQM when one is concerned about position measurements, and NISA is a feature of both. In the next subsection, we will discuss about scattering in a Bohmian universe, with the final goal to motivate and justify the development of Section 4.

3.5. The Bohmian scattering cross section

In Section 2, we modelled the scattering of a single particle in an OQM framework. On the other hand, an idealized one-particle scattering experiment in a Bohmian universe goes as follows: we have a particle with an initial position $\mathbf{x}(0)$ and in a state ψ heading towards the *scattering center*, i.e. where the potential V is localized (we take this as the origin of our Cartesian coordinate system). As the particle is assumed to be initially far away from the scattering center, we expect it to move freely. However, as it approaches the origin, the particle is influenced by the potential V; once it reaches the origin, it is scattered off and subsequently leaves the 'scattering region', i.e. roughly speaking the open set with nonzero Lebesgue measure containing $\mathbf{0} \in \mathbb{R}^3$ where the potential V markedly[115] influences the evolution of the particle. Once out of the scattering region, it moves freely up until it reaches the surface of a detector situated far away from the scattering center that encloses our scattering setup, in particular the initial position of the particle $\mathbf{x}(0)$. The detector is such that it records the **first** exit position of the

[115] The scattering region should be understood here as a purely conceptual construct such that the reader will better imagine what happens in the vicinity of the scattering center; our rigorous analysis will bear no relation to it.

particle, i.e. plainly the point on its surface where the particle hits it for the first[116] time. Now, we divide the surface of the detector in areas, and we ask ourselves the question: what is the probability that the particle will cross one of these areas for the first time, i.e. what is the *Bohmian scattering cross section*?

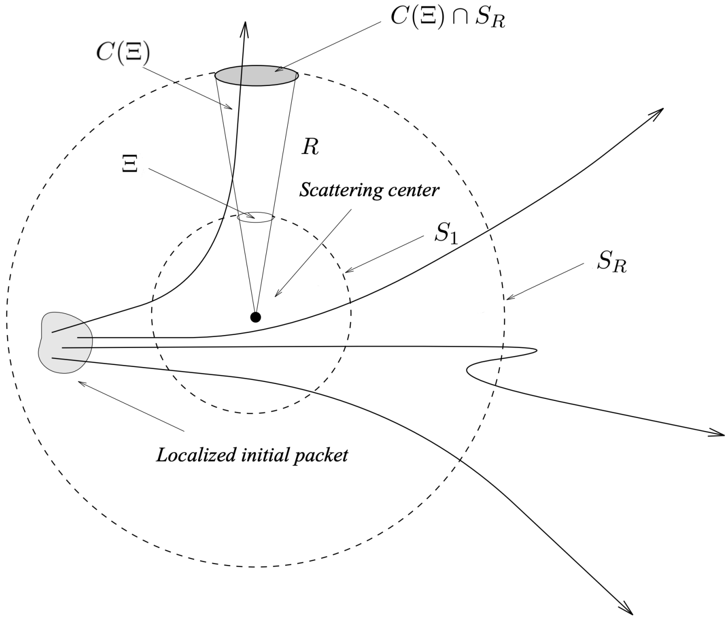

Figure 7: The same scattering setup as in Section 2, but now the particles have trajectories. Based on [DDGZ95a].

To answer sensibly to this question, we need to introduce some notation (see Figure 7).). Suppose that the wave function of the particle at all times **before** it reaches the first exit position $\psi(t)$ is supported inside the region of $\mathbb{R}^3$ that is enclosed by the detector. For simplicity, we proceed similarly as in Subsection 2.2 and take the surface of the detector to be the sphere with radius R centered at the origin $S_R \coloneqq \{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| = R\}$, such that the enclosed region is the ball $B_R \coloneqq \{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| \leq R\}$. We should then assume[117] that $\operatorname{supp} \psi(t) \subseteq B_R$, in particular $\mathbf{x}(0) \in B_R$. We further suppose that for almost

[116]There are no reasons to believe that a particle that hits the detector will not re-enter the region enclosed by it, and hit the detector again, and so on. Moreover, we assume that the detector does not influence at any time the particle prior to detection, thus ignoring any specifics concerning the sensors' mechanism.

[117]This should be taken with a grain of salt, as however skillful we are in constructing the initial state ψ, its support and the time-evolving support of $\psi(t)$ will nevertheless most likely extend way beyond B_R; we can refine our requirement by saying that the set $\operatorname{supp} \psi(t) \cap B_R^c$ is of P^{ψ_t}-measure zero (of course, if it is P^{ψ_t}-measurable).

all possible $\mathbf{x}(0)$, the particle will leave in finite time B_R, i.e. it will hit the detector's surface. Subsequently, by taking a Borel measurable set $\Xi \subseteq S_1$, we conveniently define the generalized cone

$$C(\Xi) \coloneqq \{c\mathbf{x} : c \in \mathbb{R}_0^+ \text{ and } \mathbf{x} \in \Xi\},$$

such that, say, for pairwise disjoint $\{\Xi_i\}_{i\in I}$ with $\bigcup_{i\in I} \Xi_i = S_1$, for a countable I, we have that $\{C(\Xi_i)\}_{i\in I}$ are disjoint as well, and moreover

$$C(\Xi_j) \cap S_R$$

is the j-th area of the surface of the detector, $j \in I$, and naturally the union of disjoint areas

$$\bigcup_{i\in I} (C(\Xi_i) \cap S_R) = S_R$$

gives the whole surface of the detector.

Now, define the random variable[118]

$$X_{\mathrm{FE}} : B_R^* \longrightarrow S_R$$

$$\mathbf{x} \mapsto \{\widetilde{\mathbf{x}} \in S_R : \widetilde{\mathbf{x}} = \mathbf{x}(t_{\mathrm{FE}}),\ \mathbf{x}(t) \text{ Bohmian trajectory with } \mathbf{x}(0) \coloneqq \mathbf{x}\},$$

where

$$B_R^* \coloneqq B_R \setminus \{\mathbf{x} \in B_R : \mathbf{x} \text{ is atypical}\}$$

and

$$t_{\mathrm{FE}} = \inf_{t\geq 0}\{t : \mathbf{x}(t) \in B_R^c\},$$

the definition of t_{FE} thus ensuring that the respective set[119] is a singleton, as the infima are unique. In plain words, X_{FE} maps every typical initial position $\mathbf{x} \in B_R$ to the position where the particle first exits the region enclosed by the detector, which is represented by S_R; both positions are random, according to QEH.

Also the moment of time when the particle hits the detector is random, as one well knows. Thus, the experimenter is left with adjusting R sensibly, i.e. the distance between the scattering center and the detector. Now, we know from the classical limit of BM we referred to in the previous subsection that far away from the scattering region, the Bohmian trajectories approach classical ones, i.e. straight lines. It then comes naturally to provisionally define the *Bohmian scattering cross section* associated with a particle with initial state ψ as

$$\sigma_\psi^{\mathrm{BM}}(\Xi) = \lim_{R\to\infty} P^\psi(X_{\mathrm{FE}} \in C(\Xi) \cap S_R), \tag{135}$$

[118] For a proof of measurability, see [Dau95, p.20].

[119] Note that we abused the notation, but the reader should understand that X_{FE} maps $\mathbf{x}$ to $\widetilde{\mathbf{x}}$ with the aforementioned properties, and not to the singleton $\{\widetilde{\mathbf{x}}\}$.

which unambigously represents the probability of the particle hitting the area of the detector surface $C(\Xi) \cap S_R$ for $R \to \infty$, with $\Xi \in \mathcal{B}(S_1)$.

As we take in (135) the limit $R \to \infty$, we expect that choosing another origin of our coordinate system won't influence the value of the Bohmian scattering cross section. Additionally, '$P^{\psi}(X_{\text{FE}} \in C(\Xi) \cap S_R)$' does not depend on time. Thus, in particular, we expect[120] that $\sigma_{\psi}^{\text{BM}} = \sigma_{e^{-itH}\psi}^{\text{BM}}$, for any $t \in \mathbb{R}$ (we are going to prove it in Section 4).

One might observe that (135) is of great theoretical value, but little practical one, in the sense that it is not at all clear how we can use it in calculations. Thus, our next aim is to find an explicit formula for (135). For this, further notation and concepts are needed, as we shall soon see.

The OQM interpretation of the quantum flux $\mathbf{j}$ as in (132) indicates that the quantity

$$(\mathbf{j} \cdot d\mathbf{S})\, dt \tag{136}$$

gives the probability that a particle crosses the oriented surface $d\mathbf{S}$ in the time dt, **if** (136) is nonnegative. However, knowing when $(\mathbf{j} \cdot d\mathbf{S})\, dt \geq 0$ is an ambiguous endeavour, if one starts with OQM. Contrary to OQM, BM clearly[121] implies that (136) gives the expected number of *signed crossings* through the oriented surface $d\mathbf{S}$ in the time dt [DDGZ95b].

Back to our scattering status quo. We will refer to the number of signed crossings[122] through $C(\Xi) \cap S_R$ as N^{Ξ}_{sgn}. It is also useful to introduce N^{Ξ}_{tot}, the total number of crossings, this time adding $+1$ for each crossing of the surface, may it be outward or inward. Thus, the number of outward and inward crossings is $N^{\Xi}_{+} = \frac{1}{2}(N^{\Xi}_{\text{tot}} + N^{\Xi}_{\text{sgn}})$ and $N^{\Xi}_{-} = \frac{1}{2}(N^{\Xi}_{\text{tot}} - N^{\Xi}_{\text{sgn}})$, respectively. With this notation, and having in mind the BM interpretation of (136), we have that the expected number of signed crossings N^{Ξ}_{sgn} of particles prepared in the initial state $\psi := \psi(0)$ through the area of the detector's surface $C(\Xi) \cap S_R$ is given by

$$E_{\psi}(N^{\Xi}_{\text{sgn}}) := \int_0^{\infty} \int_{C(\Xi)\cap S_R} \mathbf{j} \cdot d\mathbf{S}\, dt,$$

if, of course, we have that the expected total number of crossings is finite, i.e.

$$E_{\psi}(N^{\Xi}_{\text{tot}}) := \int_0^{\infty} \int_{C(\Xi)\cap S_R} |\mathbf{j} \cdot d\mathbf{S}|\, dt < \infty,$$

[120] However, in real world experiments, one does not have the liberty of having a detector conveniently placed at infinity. Thus it is instead expected that the Bohmian scattering cross section won't be changed by shifts in the origin that are small relative to R, and that we can virtually activate the detectors at any time we wish **before** the particle reaches it.

[121] This is a direct consequence of the fact that reasoning with trajectories lifts the inherent ambiguity of OQM regarding what it really means for a particle to hit the detector: if we do not have positions for the particles, then when and how do we know that it actually crossed a surface?

[122] Empirically, we add $+1$ for outward crossings, and -1 for inward crossings, where 'outward' and 'inward' are with respect to the orientation of the surface $d\mathbf{S}$.

where $d\mathbf{S}$ is the normal surface element of $C(\Xi) \cap S_R$.

Now we recall that for large R, the classical limit of BM predicts that the Bohmian trajectories are straight lines in the vicinity of the detector, so that the *positivity condition*

$$\mathbf{j} \cdot d\mathbf{S} \geq 0$$

is expected to hold almost everywhere on the surface of the detector (the positivity condition can be justified rigorously, see [DDGZ95a]). Thus, almost all the crossings of the detector's surface will be outward, i.e.

$$E_\psi(N_-^\Xi) \approx 0,$$

so that we can infer that

$$P^\psi(X_{\mathrm{FE}} \in C(\Xi) \cap S_R) \approx E_\psi(N_+^\Xi) \approx E_\psi(N_{\mathrm{sgn}}^\Xi) \approx E_\psi(N_{\mathrm{tot}}^\Xi). \tag{137}$$

Hence, in order to have an analytically tractable definition for the Bohmian scattering cross section, we take

$$\sigma_\psi^{\mathrm{BM}}(\Xi) := \lim_{R\to\infty} \int_0^\infty \int_{C(\Xi)\cap S_R} \mathbf{j} \cdot d\mathbf{S}\, dt.$$

Proving that in the limit $R \to \infty$, the last two approximations in (137) turn into identities, is one of the main goals of Section 4.

Remark. Since the Introduction, we touted this work as dealing only with one-particle scattering. Now we are in the position to explain this apparent limitation, as indeed, as we highlighted in Subsection 3.3, BM can be easily generalized to N-particle systems. However, the quantum flux for an N-particle system $\mathbf{j}(\mathbf{X}(t), t)$, where as before $\mathbf{X}(t) := (\mathbf{x}_1(t), \ldots, \mathbf{x}_N(t))$, loses its physical meaning. A simple reason for this is that in the case of an N-particle system we have N random times when the detector gets activated; a more rigorous justification can be found in Detlef Dürr's and Stefan Teufel's contribution to [BD04].

4. Bohmian mechanics brings acuity to mathematical scattering theory

The purpose of Section 2 was twofold: on the one hand, we tried to highlight the importance of Dollard's scattering-into-cones theorem in understanding the connection between the orthodox scattering cross section and IOAS; on the other hand, we showed how the asymptotic completeness of $\Omega_\pm$ shines some light on what we refer to in OQM as bound states (roughly some of the states that do **not** belong to $\mathfrak{D}(\Omega_\pm)$) and scattering states (the elements of $\mathfrak{R}(\Omega_-) \cap \mathfrak{R}(\Omega_+)$).

In the current section, we will revisit the same two topics from a Bohmian perspective. Subsections 4.1-4.2 are a discussion of the (free) flux-across-surfaces-theorem, the BM counterpart of Dollard's (free) scattering-into-cones theorem, while in Subsection 4.3 we will derive using BM a sufficient condition to assess whether a state has IOAS.

4.1. Setting our Bohmian intuition in mathematical terms

In Subsection 3.5, we argued heuristically that when the detector is placed far away from the scattering center, then for a particle in an initial state ψ it holds true at time[123] T that

$$E_\psi(N_+^\Xi) \approx E_\psi(N_{\text{sgn}}^\Xi) \approx E_\psi(N_{\text{tot}}^\Xi), \tag{138}$$

where we recast for convenience and generality

$$E_\psi(N_{\text{tot}}^\Xi) := \int_T^\infty \int_{C(\Xi)\cap S_R} |\mathbf{j}\cdot d\mathbf{S}|\, dt, \tag{139}$$

$$E_\psi(N_{\text{sgn}}^\Xi) := \int_T^\infty \int_{C(\Xi)\cap S_R} \mathbf{j}\cdot d\mathbf{S}\, dt, \tag{140}$$

$$E_\psi(N_+^\Xi) := \frac{1}{2}\left(E_\psi(N_{\text{sgn}}^\Xi) + E_\psi(N_{\text{tot}}^\Xi)\right), \tag{141}$$

the last two integrals being finite if and only if $E(N_{\text{tot}}^\Xi) < \infty$.

We will cement our belief in (138) by taking its limit[124] $R \to \infty$, as prescribed by the classical limit of BM, and consequently proving rigorously that

$$\lim_{R\to\infty} E_\psi(N_+^\Xi) = \lim_{R\to\infty} E_\psi(N_{\text{sgn}}^\Xi) = \lim_{R\to\infty} E_\psi(N_{\text{tot}}^\Xi), \tag{142}$$

where we recall that the Bohmian scattering cross section was defined as

$$\sigma_\psi^{\text{BM}}(\Xi) := \lim_{R\to\infty} E_\psi(N_{\text{sgn}}^\Xi). \tag{143}$$

[123] By which we mean that we pick a $T \in \mathbb{R}$ as the time the detector is activated, with the obvious proviso that this is such that the particle will cross the detector's surface at a random moment of time $\widetilde{T} > T$.

[124] Where now we can really take any $T \in \mathbb{R}$, as the detector is now 'placed at infinity'.

But before we embark in our proof of (142), notice that by proving that

$$\lim_{R\to\infty} E_\psi(N^{\Xi}_{\text{sgn}}) = \lim_{R\to\infty} E_\psi(N^{\Xi}_{\text{tot}}),$$

we have that $\lim_{R\to\infty} E_\psi(N^{\Xi}_{+})$ is automatically equal to them in view of (141), so what we really want to show is that

$$\lim_{R\to\infty}\int_T^\infty \int_{C(\Xi)\cap S_R} \mathbf{j}\cdot d\mathbf{S}\,dt = \lim_{R\to\infty}\int_T^\infty \int_{C(\Xi)\cap S_R} |\mathbf{j}\cdot d\mathbf{S}|\,dt. \tag{144}$$

Furthermore, we will restrict ourselves to a proof of (144) in the free case[125], i.e. $V = 0$, to keep this work concise and focused on the physical aspects of the (now free) flux-across-surfaces theorem. However, we will provide the reader with references for the flux-across-surfaces theorem for short- and long-range potentials at the right time; for now, bear with us, as the proof of the free flux-across-surfaces theorem requires patience with technical details.

4.2. The particle really crosses the surface of the detector

We start with the following conjecture: we expect that for an arbitrary[126] $\Xi \in \mathcal{B}(S_1)$ and an initial state[127] $\psi \in S(\mathbb{R}^m)$ to have equality between the Bohmian and the orthodox scattering cross section, i.e.

$$\sigma^{\text{BM}}_{\psi,\text{free}}(\Xi) = \sigma^{\text{OQM}}_{\psi,\text{free}}(\Xi); \tag{145}$$

we base this guess on the fact that both the limit $t\to\infty$ that appears in the definition of $\sigma^{\text{OQM}}_{\psi,\text{free}}$, as well as the limit $R\to\infty$ in $\sigma^{\text{BM}}_{\psi,\text{free}}$, aim to achieve exactly the same thing: to stipulate that our particle is crossing outwardly the surface of the detector S_R, and does not return inside the region enclosed by it B_R.

Now, in view of the Dollard's free scattering-into-cones theorem (96) for[128] $t\to\infty$, (145) turns into[129]

$$\sigma^{\text{BM}}_{\psi,\text{free}}(\Xi) = \int_{C(\Xi)} |(\mathcal{F}\psi)(\mathbf{x})|^2\, d^m x,$$

[125] To the best of our knowledge, 'the simplest' proof of the free flux-across-surfaces theorem to date was presented as part of Teufel's PhD thesis [Teu99], while the first one was given in [DGZ96], followed closely by the one in [WA97a] (we refer here only to proofs that situated the free flux-across-srufaces-theorem in a BM framework).

[126] Although all the mathematical objects we are working with accommodate a $\psi \in L^2(\mathbb{R}^m)$, the restriction to $\psi \in S(\mathbb{R}^m)$ is for mere convenience, owing to the nice properties of the Schwartz space $S(\mathbb{R}^m)$; moreover, the diagonalization of the free evolution implies that $e^{-itH_0}S(\mathbb{R}^m) \subseteq S(\mathbb{R}^m)$, a necessary condition for what follows, see Appendices C and D.

[127] By (192), $S(\mathbb{R}^m)$ is invariant under the free evolution.

[128] For brevity, from now on we will deal only with the experimentally relevant $t\to\infty$, and discard the mathematically identical, but physically insignificant $t\to-\infty$.

[129] As we are not interested anymore in denoting the momentum by the distinctive variable '$\mathbf{k}$', we drop its meaning in this section, and replace it in (96) by '$\mathbf{x}$'.

so that, if we manage to prove that

$$\lim_{R\to\infty}\int_T^\infty \int_{C(\Xi)\cap S_R} \mathbf{j}\cdot d\mathbf{S}\,dt = \int_{C(\Xi)} |(\mathcal{F}\psi)(\mathbf{x})|^2\,d^m x, \tag{146}$$

and then that

$$\lim_{R\to\infty}\int_T^\infty \int_{C(\Xi)\cap S_R} |\mathbf{j}\cdot d\mathbf{S}|\,dt = \int_{C(\Xi)} |(\mathcal{F}\psi)(\mathbf{x})|^2\,d^m x, \tag{147}$$

it follows that (144) is true as well.

We will perform one more a priori simplification: as

$$\sigma^{\mathrm{OQM}}_{\psi,\mathrm{free}}(\Xi) = \int_{C(\Xi)} |(\mathcal{F}\psi)(\mathbf{x})|^2\,d^m x, \tag{148}$$

one can see that by a shift $T' \in \mathbb{R}$ in the time at which we activate the detector T, the orthodox scattering cross section in the new regime (the activation time of the detector is now $T+T'$) is identical, i.e. the orthodox scattering cross section is invariant under shifts T' in the time at which we activate the detector. To see this, note that it is sufficient to show that for ψ in (148) the state at $t=0$, it is true for the state at $t=T\in\mathbb{R}$ that

$$\begin{aligned}\int_{C(\Xi)} |(\mathcal{F}e^{-iTH_0}\psi)(\mathbf{x})|^2\,d^m x &= \int_{C(\Xi)} |e^{-iT|\mathbf{x}|^2}\mathcal{F}\psi(\mathbf{x})|^2\,d^m x\\ &= \int_{C(\Xi)} |(\mathcal{F}\psi)(\mathbf{x})|^2\,d^m x\\ &= \sigma^{\mathrm{OQM}}_{\psi,\mathrm{free}}(\Xi),\end{aligned}$$

where we just substituted the diagonalization of the free evolution (192).

The invariance discussed above implies that if we prove (146) and (147), then $\sigma^{\mathrm{BM}}_{\psi,\mathrm{free}}$ will be invariant under shifts in the time at which we activate the detector[130] as well. Consequently, we can restrict ourselves to showing (144) for all $T\geq a$ for a fixed and arbitrary $a\in\mathbb{R}$ (or, equivalently, for $T\leq a$), as then the general result in which $T\in\mathbb{R}$ follows from the aforementioned invariance under shifts. In the further, we will then stick to $T\geq 1$, a choice that will prove its usefulness at the right time.

As we are interested in proving (146) and (147), we need to evaluate $\mathbf{j}$. However, feeding directly $e^{-itH_0}\psi$ in (132) does not seem very illuminating; instead, as we are in the free case, it comes natural to start the explicit proof with

$$e^{-itH_0}\psi(\mathbf{x}) = (4\pi i t)^{-m/2}\int_{\mathbb{R}^m} e^{i|\mathbf{x}-\mathbf{y}|^2/4t}\psi(\mathbf{y})\,d^m y, \tag{149}$$

[130] I.e. $T+T'$ replaces T in (144), but $\sigma^{\mathrm{OQM}}_{\psi,\mathrm{free}}(\Xi)$ has the same value for T and $T+T'$.

for $t \neq 0$, where the expansion above is from[131] [Tes14, p.199]; (149) provided us with a way to explicitly express $e^{-itH_0}\psi$ as part of the proof for the Dollard's free scattering-into-cones theorem, so it is definitely a good start. Besides, we further observe that combining

$$e^{i|\mathbf{x}-\mathbf{y}|^2/4t} = e^{i|\mathbf{x}|^2/4t}e^{-i\mathbf{x}\cdot\mathbf{y}/2t} + e^{i|\mathbf{x}|^2/4t}e^{-i\mathbf{x}\cdot\mathbf{y}/2t}\left(e^{i|\mathbf{y}|^2/4t} - 1\right);$$

with (149) it leads to:

$$\begin{aligned} e^{-itH_0}\psi(\mathbf{x}) &= (4\pi it)^{-m/2}e^{i|\mathbf{x}|^2/4t}\int_{\mathbb{R}^m} e^{-i\mathbf{x}\cdot\mathbf{y}/2t}\psi(\mathbf{y})\,d^m y \\ &\quad + (4\pi it)^{-m/2}e^{i|\mathbf{x}|^2/4t}\int_{\mathbb{R}^m} e^{-i\mathbf{x}\cdot\mathbf{y}/2t}\left(e^{i|\mathbf{y}|^2/4t} - 1\right)\psi(\mathbf{y})\,d^m y. \end{aligned} \tag{150}$$

The first term on the right-hand side of the identity above is

$$(4\pi it)^{-m/2}e^{i|\mathbf{x}|^2/4t}\int_{\mathbb{R}^m} e^{-i\mathbf{x}\cdot\mathbf{y}/2t}\psi(\mathbf{y})\,d^m y = (2it)^{-m/2}e^{i|\mathbf{x}|^2/4t}(\mathcal{F}\psi)\left(\frac{\mathbf{x}}{2t}\right),$$

which upon $|\cdot|^2$ and integration over the cone $C(\Xi)$ gives the orthodox scattering cross section

$$(2t)^{-m}\int_{C(\Xi)}\left|(\mathcal{F}\psi)\left(\frac{\mathbf{x}}{2t}\right)\right|^2 d^m x = \int_{C(\Xi)}|(\mathcal{F}\psi)(\mathbf{x})|^2\,d^m x = \sigma^{\mathrm{OQM}}_{\psi,\mathrm{free}}(\Xi),$$

a result that heuristically makes sense, as the 'factor' in the integrand of the second term of (150) becomes insignificant for large t, i.e. $|e^{-i\mathbf{x}\cdot\mathbf{y}/2t}\left(e^{i|\mathbf{y}|^2/4t} - 1\right)| = |e^{i|\mathbf{y}|^2/4t} - 1| \to 0$ as $t \to \infty$; however, if we stick to rigour we cannot get rid so easily of the second term of (150), so, partly for aesthetical reasons, we denote the terms by

$$\begin{aligned} \eta(\mathbf{x}, t) &\coloneqq (2\pi it)^{-m/2}e^{i|\mathbf{x}|^2/4t}(\mathcal{F}\psi)\left(\frac{\mathbf{x}}{2t}\right), \\ \mu(\mathbf{x}, t) &\coloneqq (4\pi it)^{-m/2}e^{i|\mathbf{x}|^2/4t}\int_{\mathbb{R}^m} e^{-i\mathbf{x}\cdot\mathbf{y}/2t}\left(e^{i|\mathbf{y}|^2/4t} - 1\right)\psi(\mathbf{y})\,d^m y; \end{aligned}$$

we then use brute force to compute:

$$\begin{aligned} \mathbf{j}(\mathbf{x}, t) &= 2\mathrm{Im}\left\{(e^{-itH_0}\psi(\mathbf{x}))^*\nabla(e^{-itH_0}\psi(\mathbf{x}))\right\} \\ &= 2(2t)^{-m-1}\left|(\mathcal{F}\psi)\left(\frac{\mathbf{x}}{2t}\right)\right|\mathbf{x} \\ &\quad + 2\mathrm{Im}\left\{(2t)^{-m-1}(\mathcal{F}\psi^*)\left(\frac{\mathbf{x}}{2t}\right)\nabla(\mathcal{F}\psi)\left(\frac{\mathbf{x}}{2t}\right)\right. \\ &\quad \left. +\mu^*(\mathbf{x}, t)\nabla\eta(\mathbf{x}, t) + \eta^*(\mathbf{x}, t)\nabla\mu(\mathbf{x}, t) + \mu^*(\mathbf{x}, t)\nabla\mu(\mathbf{x}, t)\right\}, \end{aligned}$$

[131] We used it already in proving Lemma C.1.

where we spared from writing with respect to η, μ the first terms in the expression for $\mathbf{j}$ and the argument of Im, respectively, to avoid clouding their meaning. Indeed, the first term in $\mathbf{j}$ is hinting at the right-hand side of (148), thus it would be enlightening to integrate it:

$$\begin{aligned}
&\lim_{R\to\infty}\int_T^\infty \int_{C(\Xi)\cap S_R} 2(2t)^{-m-1}\left|(\mathcal{F}\psi)\left(\frac{\mathbf{x}}{2t}\right)\right| \mathbf{x}\cdot\, d\mathbf{S}\, dt \\
&= \lim_{R\to\infty}\int_T^\infty \int_{C(\Xi)\cap S_R} 2(2t)^{-m-1}\left|(\mathcal{F}\psi)\left(\frac{R\boldsymbol{\omega}}{2t}\right)\right| R^m\, d\Omega\, dt \\
&= \lim_{R\to\infty}\int_{R/2T}^0 \int_{C(\Xi)\cap S_R} -|\mathbf{k}|^{m-1}\left|(\mathcal{F}\psi)(\mathbf{k})\right|\, d\Omega\, d|\mathbf{k}| \\
&= \lim_{R\to\infty}\int_0^{R/2T} \int_{C(\Xi)\cap S_R} |\mathbf{k}|^{m-1}\left|(\mathcal{F}\psi)(\mathbf{k})\right|\, d\Omega\, d|\mathbf{k}| \\
&= \int_{C(\Xi)} |(\mathcal{F}\psi)(\mathbf{k})|^2\, d^m k \\
&= \int_{C(\Xi)} |(\mathcal{F}\psi)(\mathbf{x})|^2\, d^m x \\
&= \sigma^{\mathrm{OQM}}_{\psi,\mathrm{free}}(\Xi),
\end{aligned} \tag{151}$$

where we used that: $dS = R^{m-1}\, d\Omega$, which implies $\mathbf{x}\cdot d\mathbf{S} = \mathbf{x}\cdot(\mathbf{x}/|\mathbf{x}|)\, dS = R\, dS = R^m\, d\Omega$ as $|\mathbf{x}| = R$ on $C(\Xi)\cap S_R$, together with the change to spherical coordinates $\mathbf{k} = R\boldsymbol{\omega}/2t$, such that $d|\mathbf{k}| = d|R\boldsymbol{\omega}/2t| = -R\, dt/2t^2$; in the third line from the bottom we reverted back to an integral over $C(\Xi)$ by a standard[132] procedure of integrating with respect to the spherical measure, and then we changed back the name of the variable to '$\mathbf{x}$', to avoid any confusions with the momentum (as we work in a BM framework), and then we applied Dollard's free scattering-into-cones theorem. Consequently, we denote the remainder as:

$$\begin{aligned}
\mathbf{R}_{\eta,\mu}(\mathbf{x},t) := 2\mathrm{Im}\Big\{&(2t)^{-m-1}(\mathcal{F}\psi^*)\left(\frac{\mathbf{x}}{2t}\right)\nabla(\mathcal{F}\psi)\left(\frac{\mathbf{x}}{2t}\right) \\
&+\mu^*(\mathbf{x},t)\nabla\eta(\mathbf{x},t) + \eta^*(\mathbf{x},t)\nabla\mu(\mathbf{x},t) + \mu^*(\mathbf{x},t)\nabla\mu(\mathbf{x},t)\Big\},
\end{aligned} \tag{152}$$

so that

$$\lim_{R\to\infty}\int_T^\infty \int_{C(\Xi)\cap S_R} \mathbf{j}\cdot\, d\mathbf{S}\, dt = \sigma^{\mathrm{OQM}}_{\psi,\mathrm{free}}(\Xi) + \lim_{R\to\infty}\int_T^\infty \int_{C(\Xi)\cap S_R} \mathbf{R}_{\eta,\mu}(\mathbf{x},t)\cdot\, d\mathbf{S}\, dt. \tag{153}$$

If we manage to show that

$$\lim_{R\to\infty}\int_T^\infty \int_{C(\Xi)\cap S_R} \mathbf{R}_{\eta,\mu}(\mathbf{x},t)\cdot\, d\mathbf{S}\, dt = 0, \tag{154}$$

[132] If the reader is not familiar with this topic, then she/he might find it useful to glance over [Yeh06, p.667-671].

then we are done with the first part of our proof, i.e. (146). Further observe that

$$0 \leq \left| \int_T^\infty \int_{C(\Xi)\cap S_R} \mathbf{R}_{\eta,\mu}(\mathbf{x},t) \cdot \, d\mathbf{S}\, dt \right| \leq \int_T^\infty \int_{C(\Xi)\cap S_R} |\mathbf{R}_{\eta,\mu}(\mathbf{x},t)\cdot(\mathbf{x}/|\mathbf{x}|)| \, dS\, dt,$$

so if

$$\lim_{R\to\infty} \int_T^\infty \int_{C(\Xi)\cap S_R} |\mathbf{R}_{\eta,\mu}(\mathbf{x},t)\cdot(\mathbf{x}/|\mathbf{x}|)| \, dS\, dt = 0 \tag{155}$$

is true, then also (154) holds. To show (155), it would be convenient to find an upper bound[133] $M(R,t)$ for $|\mathbf{R}_{\eta,\mu}(\mathbf{x},t)|$ on the surface $C(\Xi)\cap S_R$, for any $\Xi \in \mathcal{B}(S_1)$; the latter condition is naturally satisfied if we look directly for an upper bound for the entire S_R, as $C(\Xi)\cap S_R \subseteq C(S_1)\cap S_R = S_R$. But in which way can we upper bound $|\mathbf{R}_{\eta,\mu}(\mathbf{x},t)|$, in order to facilitate our proof? Certainly by trying to find an upper bound for its least upper bound on S_R, given the fact that $S(\mathbb{R}^m)$ is defined using the sup norm $\|\cdot\|_\infty \coloneqq \sup_{\mathbf{x}\in\mathbb{R}^m} |\cdot|$, and we also have that $\sup_{\mathbf{x}\in S_R} |\cdot| \leq \|\cdot\|_\infty$. Thus, we look for a $M(R,t)$ with the properties

$$\sup_{\mathbf{x}\in S_R} |\mathbf{R}_{\eta,\mu}(\mathbf{x},t)| \leq M(R,t),$$

$$\lim_{R\to\infty} \int_T^\infty \int_{S_R} M(R,t)\, dS\, dt = 0;$$

the last property is actually equivalent to

$$\begin{aligned} \lim_{R\to\infty} \int_T^\infty \int_{S_R} M(R,t)\, dS\, dt &= \lim_{R\to\infty} \int_T^\infty M(R,t) \int_{S_R} dS\, dt \\ &= c_1 \lim_{R\to\infty} R^{m-1} \int_T^\infty M(R,t)\, dt, \end{aligned} \tag{156}$$

for a $c_1 > 0$ for which we have a fixed value, although it is not posing any interest here. Thus, (156) hints at the shape of the upper bound

$$M(R,t) = c_{2,\varepsilon} t^{-1-\varepsilon} R^{-m+\varepsilon}, \tag{157}$$

for a $c_{2,\varepsilon} > 0$ and $\varepsilon \in (0,1)$, as then

$$\begin{aligned} \lim_{R\to\infty} \int_T^\infty \int_{S_R} M(R,t)\, dS\, dt &= c_1 c_{2,\varepsilon} \lim_{R\to\infty} R^{m-1} R^{-m+\varepsilon} \int_T^\infty t^{-1-\varepsilon}\, dt \\ &= \frac{c_1 c_{2,\varepsilon}}{\varepsilon T^\varepsilon} \lim_{R\to\infty} R^{-1+\varepsilon} = 0, \end{aligned}$$

[133]From $|\mathbf{R}_{\eta,\mu}(\mathbf{x},t)\cdot(\mathbf{x}/|\mathbf{x}|)| \leq |\mathbf{R}_{\eta,\mu}(\mathbf{x},t)|$. Observe that we actually use $|\cdot|$ to denote two different things: in the case of $\mathbf{R}_{\eta,\mu}(\mathbf{x},t)\cdot(\mathbf{x}/|\mathbf{x}|)$, it is the absolute value of a complex number (Euclidean norm on $\mathbb{C}$), while in the case of $\mathbf{R}_{\eta,\mu}(\mathbf{x},t)$, as well as $\mathbf{x}$ and $\mathbf{y}$, by $|\cdot|$ we mean the Euclidean norm on $\mathbb{C}^m$; many similar situations arise in the subsequent paragraphs, however we will **not** distinguish between them as the context is sufficient to infer about which $|\cdot|$ we are talking about.

where we know that $T^\varepsilon > 0$ as we assumed a while ago that $T \geq 1$.

Finally, (146) follows if we succeed in proving that there exists an M of the shape (157). Having the latter in the back of our mind, we glance once more over the remainder (152) and the definition of μ and η, and after splitting each and every term inside $\mathrm{Im}\{\dots\}$ with the help of the homogeneity property $|c\mathbf{v}| = |c||\mathbf{v}|$ for a $c \in \mathbb{C}$ and $\mathbf{v} \in \mathbb{C}^m$, and using the common sense relationship $|\mathrm{Im}\{\cdot\}| \leq |\cdot|$, we are led to show that:

$$|(\mathcal{F}\psi^*)(\mathbf{x}/2t)| \leq \gamma(p)(2t/R)^p, \tag{158}$$

$$|(\nabla\mathcal{F}\psi)(\mathbf{x}/2t)| \leq \gamma(p)(2t/R)^p, \tag{159}$$

$$|\eta^*(\mathbf{x},t)| \leq \gamma(p)(2t)^{-m/2}(2t/R)^p, \tag{160}$$

$$|\nabla\eta(\mathbf{x},t)| \leq \gamma(p)(2t)^{-m/2}(2t/R)^p, \tag{161}$$

$$|\mu^*(\mathbf{x},t)| \leq \gamma(p)(2t)^{-m/2-1}(2t/R)^p, \tag{162}$$

$$|\nabla\mu(\mathbf{x},t)| \leq \gamma(p)(2t)^{-m/2-1}(2t/R)^p, \tag{163}$$

with $\mathbf{x} \in S_R$, for suitable $p \in \mathbb{R}_0^+$ and $\gamma(p) \in \mathbb{R}^+$ (which we will justify soon), as then[134]

$$\begin{aligned}\sup_{\mathbf{x}\in S_R} |\mathbf{R}_{\eta,\mu}(\mathbf{x},t)| &\leq 2\{\gamma^2(p)(2t)^{-m-1}(2t/R)^{2p} + \dots + \gamma^2(p)(2t)^{-m-1}(2t/R)^{2p}\} \\ &= 12\gamma^2(p)(2t)^{-m-1}(2t/R)^{2p},\end{aligned}$$

and by setting $p = (m-\varepsilon)/2$ for an $\varepsilon \in (0,1)$, where $p > 0$ as $m \geq 1$, we obtain the promised upper bound

$$\sup_{\mathbf{x}\in S_R} |\mathbf{R}_{\eta,\mu}(\mathbf{x},t)| \leq 12\gamma^2((m-\varepsilon)/2)2^{-1-\varepsilon}t^{-1-\varepsilon}R^{-m+\varepsilon}$$

if we take $c_{2,\varepsilon} := 12\gamma^2((m-\varepsilon)/2)2^{-1-\varepsilon}$.

Let us explain why there exists a $\gamma : \mathbb{R}_0^+ \longrightarrow \mathbb{R}^+$ for which (158)-(163) are true. A first thing to notice is that it suffices to restrict ourselves to defining γ for $p \in \mathbb{N}_0$, as if $2t/R < 1$, then $(2t/R)^p \leq (2t/R)^q$ if $p := \lceil q \rceil$, and similarly for $2t/R \geq 1$, it is true that $(2t/R)^p \leq (2t/R)^q$ if $p := \lfloor q \rfloor$. Consequently, if we know $\gamma(p)$ for all $p \in \mathbb{N}_0$, then in the case $2t/R < 1$ we can conveniently define γ on $(p-1,p)$ for $p \neq 0$ as e.g. the constant mapping $(p-1,p) \ni x \mapsto 2\gamma(p)$, thus obtaining γ for all $x \in \bigcup_{p'\in\mathbb{N}}(p'-1,p') = \mathbb{R}^+ \setminus \mathbb{N}$ (constructing a suitable γ for the case $2t/R \geq 1$ given $\gamma(p)$ for all $p \in \mathbb{N}_0$ is similar[135]).

Next, we turn our attention to (158). We assumed that $\psi(\cdot) \in S(\mathbb{R}^m)$, so also $\psi^*(\cdot) \in S(\mathbb{R}^m)$, as well as $\psi^*(\cdot/2t) \in S(\mathbb{R}^m)$, as one can easily check; additionally it

[134] Here we firstly used that $|\mathrm{Im}\{\cdot\}| \leq |\cdot|$, and subsequently we applied the triangle inequality.

[135] Although we took $c_{2,\varepsilon} := 12\gamma^2((m-\varepsilon)/2)2^{-1-\varepsilon}$ for an $\varepsilon \in (0,1)$, we can, by the way we defined γ, take the supremum over ε and thus obtain a c_2 to replace $c_{2,\varepsilon}$ in (157).

holds true that $\mathcal{F}S(\mathbb{R}^m) \subseteq S(\mathbb{R}^m)$ (via the definition of the Fourier transform), so $(\mathcal{F}\psi^*)(\cdot/2t) \in S(\mathbb{R}^m)$. We can then use effectively the definition[136] of $S(\mathbb{R}^m)$ (in fact, an equivalent[137] condition to the one used in (201)) to upper bound our term:

$$|(\mathcal{F}\psi^*)(\mathbf{x}/2t)| \leq \frac{C_{p,\mathbf{0}}}{(1+|\mathbf{x}|)^p}, \tag{164}$$

for a $C_{p,\mathbf{0}} > 0$, and we observe that in fact

$$|(\mathcal{F}\psi^*)(\mathbf{x}/2t)| \leq C_{p,\mathbf{0}} \frac{(2t)^p}{|\mathbf{x}|^p}, \tag{165}$$

as[138] $t \geq 1$ and $(1+|\mathbf{x}|)^p \geq |\mathbf{x}|^p$.

In particular, (165) holds for any $\mathbf{x} \in S_R$, for which $|\mathbf{x}| = R$, thus proving (158). In conclusion, for any $p \in \mathbb{N}_0$ we may define γ_1 as the mapping $p \mapsto C_{p,\mathbf{0}}$.

Next, one can show easily that $|(\nabla\mathcal{F}\psi)(\mathbf{x}/2t)| \in S(\mathbb{R}^m)$, so by proceeding identically as above we obtain $\gamma_2(p)$ for $p \in \mathbb{N}_0$. Similarly, as $(\mathcal{F}\psi)(\cdot/2t) \in S(\mathbb{R}^m)$, one may multiply its equivalent of (165) with $(2\pi t)^{-m/2}$, thus obtaining (161), so we can define γ_3; by following the same steps, we can bound $|\nabla\eta(\mathbf{x},t)|$ and get γ_4.

Now, in the case of the left-hand sides of (162) and (163), respectively, it is not obvious at all whether we can identify any of their parts as elements of $S(\mathbb{R}^m)$, hence we need another strategy to prove the existence of γ_5 and γ_6; after we do it, we can set $\gamma(p) := \max\{\gamma_i(p)\}_{i=1}^6$ for $p \in \mathbb{N}_0$, while for $p \in \mathbb{R}^+ \setminus \mathbb{N}$ we already constructed γ, so (146) is proven.

Let us inspect μ^* once again, also keeping an eye on what we want to show, i.e. (162). We see that the factor $e^{-i\mathbf{x}\cdot\mathbf{y}/2t}$ is the most 'accessible' part of the integrands, therefore we might 'force' it into a differential form and use integration by parts. We fix $p \in \mathbb{N}_0$, and then express

$$e^{-i\mathbf{x}\cdot\mathbf{y}/2t} = i^p \left(\frac{2t}{|\mathbf{x}|}\right)^p \left\{\left(\frac{\mathbf{x}}{|\mathbf{x}|}\cdot\nabla_{\mathbf{y}}\right)^p e^{-i\mathbf{x}\cdot\mathbf{y}/2t}\right\},$$

introduce the notation $D[f(\mathbf{x},\mathbf{y})] := (\mathbf{x}\cdot\nabla_{\mathbf{y}}/|\mathbf{x}|)f(\mathbf{x},\mathbf{y})$, and plug the expression above in the formula for μ, and use that $|\mu^*| = |\mu|$ to upper bound:

$$\begin{aligned}|\mu(\mathbf{x},t)| &= (4\pi t)^{-m/2}\left|\int_{\mathbb{R}^m}\left(\frac{2t}{|\mathbf{x}|}\right)^p D^p[e^{-i\mathbf{x}\cdot\mathbf{y}}/2t](e^{i|\mathbf{y}|^2/4t}-1)\psi(\mathbf{y})\,d^my\right| \\ &\leq (2\pi t)^{-m/2}\left(\frac{2t}{|\mathbf{x}|}\right)^p \int_{\mathbb{R}^m}\left|D^p\left[(e^{i|\mathbf{y}|^2/4t}-1)\psi(\mathbf{y})\right]\right| d^my,\end{aligned} \tag{166}$$

[136]We also introduce the notation: $\boldsymbol{\alpha} := (\alpha_1,\dots,\alpha_m)$ and $\mathbf{x} := (x_1,\dots,x_m)$.

[137]I.e. for any $N \in \mathbb{N}$ and any $\boldsymbol{\alpha} \in \mathbb{N}_0^m$ there is a $C_{N,\boldsymbol{\alpha}} > 0$ such that $|\partial_{\boldsymbol{\alpha}} f(\mathbf{x})| \leq C_{N,\boldsymbol{\alpha}}/(1+|\mathbf{x}|)^N$ (we use it with $\alpha := \mathbf{0}$ and $N := p$).

[138]The inequality above is the justification for our restriction $T \geq 1$, and we remind the reader that we prove our result for any $t \geq T$, as specified by (146) and (147).

where we used integration by parts for p times, and the fact that $(4\pi t)^{-m/2} < (2\pi t)^{-m/2}$ is true for $t \geq 1$.

We look at the last line of (166) and see that if we manage to show that

$$\int_{\mathbb{R}^m} \left| D^p[(e^{i|\mathbf{y}|^2/4t} - 1)\psi(\mathbf{y})] \right| d^m y \leq \frac{\varsigma}{2t}, \tag{167}$$

for a $\varsigma > 0$, then we can conclude that indeed[139]

$$\begin{aligned} |\mu(\mathbf{x},t)| &\leq (2\pi t)^{-m/2} \left(\frac{2t}{|\mathbf{x}|}\right)^p \int_{\mathbb{R}^m} \left| D^p[(e^{i|\mathbf{y}|^2/4t} - 1)\psi(\mathbf{y})] \right| d^m y \\ &\leq \varsigma \pi^{-m/2} (2t)^{-m/2-1} \left(\frac{2t}{|\mathbf{x}|}\right)^p \\ &= \varsigma \pi^{-m/2} (2t)^{-m/2-1} \left(\frac{2t}{R}\right)^p, \end{aligned}$$

which tells us that we can set γ_5 to be the mapping $p \mapsto \varsigma\pi^{-m/2}$, of course once we showed that there is a $\varsigma > 0$ with the property (167).

Let us take a closer look at D. As we apply it p times to $(e^{i|\mathbf{y}|^2/4t} - 1)\psi(\mathbf{y})$, we will obtain many (t^{-n})-dependent terms from the exponent $i|\mathbf{y}|^2/4t$, where $n \leq p$ is a natural number. However, in order to pull the (t^{-n}) terms out of the integral, we need to expand the integrand in an orderly fashion; as it is, D contains '∇', and we know from univariate calculus that the Leibniz rule

$$\frac{d^p}{dx^p}(fg) = \sum_{j=0}^{p} \binom{p}{j} f^j g^{p-j}$$

provides us with a way to expand the p-order derivatives d^p/dx^p of a product of functions fg. One can easily show that D satisfies its own Leibniz rule, i.e. we have that

$$\begin{aligned} D^p[(e^{i|\mathbf{y}|^2/4t} - 1)\psi(\mathbf{y})] &= \sum_{j=0}^{p} \binom{p}{j} D^j[e^{i|\mathbf{y}|^2/4t} - 1] D^{p-j}[\psi(\mathbf{y})] \\ &= (e^{i|\mathbf{y}|^2/4t} - 1) D^p[\psi(\mathbf{y})] + \sum_{j=1}^{p} \binom{p}{j} D^j[e^{i|\mathbf{y}|^2/4t}] D^{p-j}[\psi(\mathbf{y})], \end{aligned}$$

where to obtain the second line we observed that $D^j[e^{i|\mathbf{y}|^2/4t} - 1] = D^j[e^{i|\mathbf{y}|^2/4t}]$ for any $j \in \{1, \ldots, p\}$, and we also set $D^0 \coloneqq \mathbb{I}$; consequently, by applying the triangle inequality we may upper bound

$$\left| D^p[(e^{i|\mathbf{y}|^2/4t} - 1)\psi(\mathbf{y})] \right| \leq \frac{|\mathbf{y}|^2}{4t} |D^p[\psi(\mathbf{y})]| + \left| \sum_{j=1}^{p} \binom{p}{j} D^j[e^{i|\mathbf{y}|^2/4t}] D^{p-j}[\psi(\mathbf{y})] \right|,$$

[139] Remember that we are interested in (162) for $\mathbf{x} \in S_R$, so $|\mathbf{x}| = R$.

where we used the simple property $|e^{i|\mathbf{y}|^2/4t}-1| \leq |\mathbf{y}|^2/4t$ to get a t^{-1} dependent term, in view of (167). Now, in order to expose the other t^{-n} terms in the right-hand side of the inequality above, we will perform a bold step: we will expand each and every term using the Leibniz rule for the powers of D. In order to keep track of the indices that depend on other indices, it is convenient to borrow the multi-index notation we used to define $S(\mathbb{R}^m)$, such that we can efficiently write

$$\left|D^p[(e^{i|\mathbf{y}|^2/4t}-1)\psi(\mathbf{y})]\right| \leq C\left\{\sum_{\substack{\boldsymbol{\alpha}:1\leq|\boldsymbol{\alpha}|\leq p\\ \boldsymbol{\beta}:|\boldsymbol{\beta}|=p-|\boldsymbol{\alpha}|}}(2t)^{-|\boldsymbol{\alpha}|}|\mathbf{y}^{\boldsymbol{\alpha}}\partial_{\mathbf{y}}^{\boldsymbol{\beta}}\psi(\mathbf{y})| + (2t)^{-1}\sum_{1\leq|\boldsymbol{\beta}|\leq p}|y^2\partial_{\mathbf{y}}^{\boldsymbol{\beta}}\psi(\mathbf{y})|\right\},$$

where we collected in a $C>0$ all the ensuing constants that are not relevant for the shape of the right-hand side of (167).

By observing that $(2t)^{-|\boldsymbol{\alpha}|} \leq (2t)^{-1}$ for our restriction $t \geq 1$, so

$$\left|D^p[(e^{i|\mathbf{y}|^2/4t}-1)\psi(\mathbf{y})]\right| \leq C(2t)^{-1}\left\{\sum_{\substack{\boldsymbol{\alpha}:1\leq|\boldsymbol{\alpha}|\leq p\\ \boldsymbol{\beta}:|\boldsymbol{\beta}|=p-|\boldsymbol{\alpha}|}}|\mathbf{y}^{\boldsymbol{\alpha}}\partial_{\mathbf{y}}^{\boldsymbol{\beta}}\psi(\mathbf{y})| + \sum_{1\leq|\boldsymbol{\beta}|\leq p}|y^2\partial_{\mathbf{y}}^{\boldsymbol{\beta}}\psi(\mathbf{y})|\right\},$$

we obtain the desired form by integrating over $\mathbb{R}^m$ both sides of the inequality above (we know that all the integrals on the right-hand side are finite as for any multi-indices $\boldsymbol{\alpha}$, $\boldsymbol{\beta} \in \mathbb{N}_0^m$, $\mathbf{y}^{\boldsymbol{\alpha}}\partial_{\mathbf{y}}^{\boldsymbol{\beta}}\psi(\mathbf{y}) \in S(\mathbb{R}^m)$ because[140] $\psi \in S(\mathbb{R}^m)$, and we have that $S(\mathbb{R}^m) \subseteq L^1(\mathbb{R}^m)$). This completes the proof of (167), and implies (162).

And lastly, proving (163) is similar, as acting with ∇ on μ will lead to terms where, modulo constants, $\psi(\mathbf{y})$ is replaced by $\mathbf{y}\psi(\mathbf{y})$, so then for any $p \in \mathbb{N}_0$ we will have to do $p+1$ integrations by parts to upper bound $|\nabla\mu(\mathbf{x},t)|$ on S_R; we thus obtain γ_6 for $\mathbb{N}_0^+$, and then we are done with determining $\gamma : \mathbb{R}_0^+ \mapsto \mathbb{R}^+$.

To recapitulate, we established that (146) follows if (158)-(163) are valid; in view of the fact that we just determined γ, we can conclude that indeed (146) is true.

Fortunately, (147) is immediate, as we have that

$$\begin{aligned}\int_T^\infty\int_{C(\Xi)\cap S_R}\mathbf{j}\cdot d\mathbf{S}\,dt &\leq \int_T^\infty\int_{C(\Xi)\cap S_R}|\mathbf{j}\cdot d\mathbf{S}|\,dt\\ &\leq \int_T^\infty\int_{C(\Xi)\cap S_R}2(2t)^{-m-1}\left|(\mathcal{F}\psi)\left(\frac{\mathbf{x}}{2t}\right)\right||\mathbf{x}\cdot d\mathbf{S}|\,dt+\\ &+\int_T^\infty\int_{C(\Xi)\cap S_R}|\mathbf{R}_{\eta,\mu}(\mathbf{x},t)\cdot(\mathbf{x}/|\mathbf{x}|)|\,dS\,dt,\end{aligned} \tag{168}$$

[140]We abused the notation by refeering to '$\mathbf{y}^{\boldsymbol{\alpha}}\partial_{\mathbf{y}}^{\boldsymbol{\beta}}\psi(\mathbf{y})$' as an element of $S(\mathbb{R}^m)$, but the reader should have in mind the map pointwisely defined as such.

and, as $|\mathbf{x} \cdot d\mathbf{S}| = \mathbf{x} \cdot d\mathbf{S}$ if $\mathbf{x} \in C(\Xi) \cap S_R$ and $d\mathbf{S}$ is the oriented surface element of $C(\Xi) \cap S_R$, by taking the limit $R \to \infty$ in (168) and substituting (146) and (151) we are done, as then (147) follows by the squeeze theorem.

We now collect the physically relevant (147) and (146) into the theorem:

Theorem 4.1 (The free flux-across-surfaces-theorem)**.** *For a $\psi \in S(\mathbb{R}^m)$ and a set $\Xi \in \mathcal{B}(S_1)$ that generates a surface of the detector $C(\Xi) \cap S_R$, the Bohmian and orthodox scattering cross sections $\sigma^{BM}_{\psi,free}(\Xi)$ and $\sigma^{OQM}_{\psi,free}(\Xi)$, respectively, are equal with*

$$\lim_{R\to\infty} \int_T^\infty \int_{C(\Xi)\cap S_R} |\mathbf{j} \cdot d\mathbf{S}|\, dt.$$

The interested reader might find the proof of the flux-across-surfaces theorem for short- and long-range potentials in [WA97b] and [WA97a], respectively.

Thus, Theorem 4.1 formalizes the prediction of BM that the particle crosses the surface of the detector only once and heads outwardly, as long as the detector is placed far away from the scattering center. To contrast, we repeat that in OQM the treatment of the above problem, i.e. answering the question 'is the particle crossing the surface only once?', is quite vague, and relies on the unjustified presumption that if one waits long enough, the particle will move outwardly and not return. This strengthens our belief that assigning a collection of (random) positions to the particle may help us understand various quantum phenomena and circumvent some of the ambiguous assumptions of OQM at the same time.

4.3. A Bohmian sufficient condition for incoming and outgoing asymptotic states

Theorem 4.1 may be seen as a consequence of the positivity condition '$\mathbf{j} \cdot d\mathbf{S} \geq 0$ far away from the detector' we discussed in Subsection 3.5. In view of the theoretical importance of the flux-across-surfaces theorem, we will further use the positivity condition of BM to derive a sufficient condition to discriminate whether a given state has IOAS or not.

Take $\{t_n\}_{i=0}^{\infty}$ a real sequence with[141] $t_0 = 0$ that further satisfies[142] $\lim_{n\to\infty} t_n = \infty$, for which we write $\psi_n := e^{-it_nH}\psi$ for a state $\psi \in L^2(\mathbb{R}^m)$. We will denote in the following by $\mathbf{j}^{\psi_n}$ the quantum flux to stress the fact that it depends on the wave function per (132), and then ultimately on $n \in \mathbb{N}$. Thus, if BM is a good theory, it is natural[143] to presume

[141] Although we will stick to our tacit convention of (almost) always denoting the initial state by ψ.

[142] Once again we restrict ourselves to talking only about states that have IAS, as the case of states that have OAS is identical from a mathematical point of view.

[143] We believe though that, besides (169), one might find many other heuristic conditions that may be checked rigorously to be corresponding to (some of) the elements of $\mathfrak{R}(\Omega_\pm)$.

that a state for which the positivity condition

$$\lim_{n\to\infty} \mathbf{j}^{\psi_n} \cdot d\mathbf{S} \geq 0 \tag{169}$$

is true for any $R > 0$, where $d\mathbf{S}$ is the oriented surface element of S_R, is also a state that has IAS, i.e. it is an element of $\mathfrak{R}(\Omega_+)$. But in order to check this rigorously, we need to transform (169) further using some heuristical arguments.

Now, as we know that $d\mathbf{S} = (\mathbf{x}/|\mathbf{x}|)\, dS$, (169) is equivalent to requiring that:

$$\lim_{n\to\infty} \mathbf{j}^{\psi_n} \cdot \mathbf{x} \geq 0 \tag{170}$$

for any $R > 0$ and any $\mathbf{x} \in \mathbb{R}^m$ with $|\mathbf{x}| = R$. In fact, by recasting the definition for the ψ_n-dependent quantum flux

$$\mathbf{j}^{\psi_n}(\mathbf{x}, t) \coloneqq 2\mathrm{Im}\left\{\psi_n^*(\mathbf{x}, t)\nabla\psi_n(\mathbf{x}, t)\right\},$$

we see that

$$\mathbf{j}^{\psi_n}(\mathbf{x}, t) \cdot \mathbf{x} \coloneqq 2\mathrm{Im}\left\{\psi_n^*(\mathbf{x}, t)(\mathbf{x} \cdot \nabla)\psi_n(\mathbf{x}, t)\right\}. \tag{171}$$

The '$\mathbf{x} \cdot \nabla$' in the equation above is definitely reminescent of the composition XP; however, we remember that XP cannot be self-adjoint, so the correct Weyl quantization of the monomial xp is $\frac{1}{2}(XP + PX)$, and indeed by substituting $\phi_n^1 = \mathrm{Re}\{\psi_n\}$ and $\phi_n^2 = \mathrm{Im}\{\psi_n\}$ in

$$2\mathrm{Im}\left\{\psi_n^*(\mathbf{x}, t)(\mathbf{x} \cdot \nabla)\psi_n(\mathbf{x}, t)\right\},$$

and

$$\psi_n^*(\mathbf{x}, t)(XP + PX)\psi_n(\mathbf{x}, t), \tag{172}$$

it follows after some standard calculations that they are equal. In turn equation (172) hints of an expected value, a suspicion that turns out to be true simply if we integrate it; thus, we can naturally require that our states ψ are such that

$$\lim_{n\to\infty} \int_{\mathbb{R}^m} \mathbf{j}^{\psi_n} \cdot \mathbf{x}\, d^m x \geq 0, \tag{173}$$

owing to the fact that we imposed (170) to hold simultaneously for any $\mathbf{x} \in S_R$, where $R > 0$ is arbitrary.

By defining $M \coloneqq XP + PX$ for a suitable domain (see [Teu99, p.66-p.67] for all the technical details we omit), the condition (173) can then be rewritten as

$$\lim_{n\to\infty} \langle \psi_n, M\psi_n \rangle \geq 0. \tag{174}$$

As $\mathfrak{D}(M)$ was chosen such that we can decompose the identity operator as $\mathbb{I} = P_+ + P_-$, where P_+ and P_- are the projections on the positive and negative eigenspaces, respectively, in view of (174) we in fact may directly impose that $\psi \in L^2(\mathbb{R}^m)$ should be such that

$$\lim_{n\to\infty} \|P_-\psi_n\| = 0 \iff \lim_{n\to\infty} \|P_+\psi_n - \psi_n\| = 0. \tag{175}$$

And indeed, for such a $\psi \in L^2(\mathbb{R}^m)$ for which (175) holds, we have that $\psi \in \mathfrak{R}(\Omega_+)$ (see [DT00, p.12-p.14] for the proof), thus confirming our BM-mediated conjecture that they are in fact states that have IAS.

Discussion and concluding remarks

In this thesis, we aimed to make a case for Bohmian insights into mathematical scattering theory, albeit restricted to phenomena related to a single spinless nonrelativistic particle. But in order to do so, a bird's eye view over the rudiments of OQM was necessary. Hence, in Section 1, we strived to construct OQM both rigorously and intuitively starting from very general[144] assumptions; this led to the so-called 'axioms of OQM'. In brief, they tell us that: the states of a quantum system described using OQM are elements of a Hilbert space with certain characteristics (Axiom 1); an OQM observable is a self-adjoint operator (Axiom 1), and we can construct it starting from CM observables (Axiom 2); the expected value of a CM observable in a quantum system is linked to the corresponding OQM observable (Axiom 3); in OQM, the state of a quantum system 'collapses' to an eigenfunction of an OQM observable when we perform (repeated) **measurements** of the CM observable in the quantum system (Axiom 4); the time evolution of states is given by the time-dependent Schrödinger equation, which links it to the OQM observable corresponding to the total energy CM observable (Axiom 5).

In order to justify the first three axioms, in Subsections 1.1-1.2 we provided, in parallel, a rigorous derivation of the momentum and position operators for two underlying Hilbert spaces, $L^2(\mathbb{R})$ ('a particle living on the real axis') and $L^2([0, 2\pi])$ ('a particle living on a circle'). In particular, Axiom 2 and Axiom 3 hint that one might observe, at least on average, CM-specific behaviour even in a quantum system modelled via OQM, a lead that we pursued in Subsection 1.5, with positive results. Then, in Subsection 1.6, we included a discussion of Heisenberg's uncertainty principle; although indispensable when one talks about OQM, in this work the principle is even more central, as it appears to forbid the very development of BM.

After laying down the basics of OQM, in Subsection 1.7 we turned our attention to validating it from the perspective of special relativity and Bell's theorem. Namely, we checked whether our theory forbids informational superluminal action between spacelike separated events[145] (as imposed by the principle of causality in special relativity), and subsequently manifests noninformational superluminal action between spacelike separated events[146] (as mandated by Bell's theorem). While dealing with the latter issue, we provided a 'proof' of Bell's theorem using Bell's inequality (65), and then emphasized its conclusion: any theory about the Nature should be such that NISA manifests.

In Section 2, we introduced the orthodox mathematical scattering theory necessary to

[144]The most notorious assumptions in the development of Section 1 are the Born's rule, the de Broglie hypothesis and Planck's relation.

[145]The acronym we used is 'ISA'.

[146]With the acronym 'NISA'.

model a single spinless nonrelativistic particle. We started with touting the Möller wave operators $\Omega_{\pm}$ as the mathematical objects that fully capture OQM's take on scattering: in Subsection 2.1 we derived them using a heuristic of OQM ('the particle will essentially hit the detector's surface if one waits long enough'). However, as they are abstract constructs, with no obvious relationships with empirical quantities, in Subsection 2.2 we introduced the orthodox scattering cross section $\sigma_{\psi}^{\mathrm{OQM}}$ as the essential empirical quantity in any OQM-modelled scattering experiment, promising a connection with $\Omega_{\pm}$ at a latter stage, when their properties will be better understood. Hence, in Subsection 2.3 we studied their intrinsic properties, i.e. the ones that arise solely from their construction and are independent of our choice of potential V (collected in Lemma 2.1).

Nonetheless, it might well happen that the domain of the wave operators $\mathfrak{D}(\Omega_{\pm})$ is trivial for some V, hence we proved Cook's method (Theorem 2.2), which provided us with (87), a V-dependent sufficient condition for a state to be[147] in the domain of $\mathfrak{D}(\Omega_{\pm})$. But if $\Omega_{\pm}$ are nontrivial, one can use Enss' method to prove their (asymptotic) completeness, i.e. one can use them to classify, roughly speaking, the elements of the underlying Hilbert space in scattering and bound states, as presented in Subsection 2.5. And finally, in Subsection 2.6 we established the link between $\Omega_{\pm}$ and $\sigma_{\psi}^{\mathrm{OQM}}$ via Dollard's scattering-into-cones theorem (Theorem 2.4) and the formulae (101).

As the reader might have observed, we stressed 'measurements' in the first paragraph of the current section. This has to do with the fact that Axiom 4 leads to the measurement problem, an issue that motivated many physicists to question OQM, and subsequently to construct other interpretations of QM, the most relevant for the current work being BM. Thus, animated by the same motivation, in Subsection 3.1 we presented experimental data confirming that it is possible to assign trajectories to particles forming a quantum system; subsequently, in Subsections 3.2 and 3.3 we provided a derivation of BM using symmetry arguments, pointing along the way to the similarities and differences between this new theory and CM. Then, in Subsection 3.4, we stated QEH, which is the means by which BM becomes probabilistic; we highlighted that QEH implies Born's rule and the Bohmian version of Heisenberg's uncertainty principle, and it is in fact a well-grounded theorem, thus concluding that BM seems to have rigorous foundations than OQM. In the same subsection, we also mentioned that BM is such that NISA manifests, in consequence it is a theory in agreement with Bell's theorem. Lastly, in Subsection 3.5 we introduced the rigorously justified positivity condition (for the quantum flux) as the Bohmian counterpart to OQM's heuristic 'the particle will essentially hit the detector's surface if one waits long enough', and consequently defined the Bohmian scattering cross section $\sigma_{\psi}^{\mathrm{BM}}$.

[147] I.e. to be an IOAS.

We saw that BM is intrinsically connected with acuity, as it models a particle by assigning to it a (random) position. Accordingly, in Section 4 we presented Bohmian insights into the concepts introduced in Section 2. We provided the reader with Teufel's proof of the free flux-across-surfaces theorem (Theorem 4.1), the BM counterpart of OQM's free[148] Dollard's scattering-into-cones theorem, which implies that[149] $\sigma^{\mathrm{BM}}_{\psi,\mathrm{free}} = \sigma^{\mathrm{OQM}}_{\psi,\mathrm{free}}$, a further justification for the positivity condition. We start to see a pattern, so in Subsection 4.3 we further use the positivity condition to derive a sufficient condition for a state to have IOAS, i.e. to be an element of $\mathfrak{R}(\Omega_{\pm})$.

To conclude, in this work we argued that **Bohmian mathematical scattering theory** has credibility as a field of research, in view of its numerous connections to results of orthodox mathematical scattering theory, and ultimately as the predictions of BM agree in many cases to the ones of OQM. Additionally, we believe that continued research into Bohmian mathematical scattering theory will further clarify the ambiguities in the physical meaning of some of the results in orthodox scattering theory, as illustrated in Subsection 4.3.

[148]But it nevertheless extends to short- and long-range potentials as well.

[149]For some mild conditions on V and ψ.

Future work

We stressed many times that this work is addressing the modelling of the scattering of a single particle. We specified in Subsection 3.5 that for a N-particle system, the quantum flux is losing its physical meaning, so it would be worth finding a new mathematical object to represent the crossing probabilities of the scattered particles. An idea in this direction is presented in Teufel's and Dürr's contribution to [BD04], where they use insights from statistical physics to connect the Bohmian trajectories with the required probabilities.

We also restricted ourselves to a nonrelativistic treatment. When it comes to a quantum system where relativistic effects are significant, we do not (yet?) have a fully coherent relativistic BM, as e.g. there is no consensus on how to model the positrons (see the discussion at the end of [Tum18]). Nevertheless, some of the proposals for a relativistic BM, such as the one in [DGN$^+$14], are mathematically very interesting, hence worth investigating further from the perspective of mathematical physics.

Acknowledgments

First of all, I would like to thank my two supervisors, dr. Marcello Seri and Prof. dr. Diederik Roest, for guiding me through this interesting research project.

Secondly, nothing would have been possible without Ariadna Albors Zumel's constant encouragement and technical support, for which I am grateful.

A warm thank you to Imogen Leaning for patience and attention to detail.

Appendix

A. Hilbert spaces, self-adjoint operators and functional calculus via the spectral theorem for self-adjoint operators

A complex Hilbert space is a quadruple $(\mathfrak{H}, +, \cdot, \langle\cdot,\cdot\rangle)$ with the specifications: $\mathfrak{H}$ is a set such that the triple $(\mathfrak{H}, +, \cdot)$ is a complex linear space, which is also complete with respect to the norm induced by the inner product in the standard[150] way: $\|\cdot\|_{\mathfrak{H}} := \sqrt{\langle\cdot,\cdot\rangle_{\mathfrak{H}}}$.

As we now have a mathematical object consisting of a set and three maps (the Hilbert space), the next step would be to study the maps between Hilbert spaces and sets with various properties; the most useful for our analysis turn out to be the *linear operators*, i.e. (in this work) maps of the form[151]

$$A : \mathfrak{D}(A) \subseteq \mathfrak{H} \longrightarrow \mathfrak{H},$$

which are linear, with $\mathfrak{D}(A)$ a linear subspace of $\mathfrak{H}$.

As we mentioned in Section 1, we require $\mathfrak{H}$ to be *separable*[152], as this is equivalent with the existence of a countable orthonormal basis [DT09, p.255]. This ensures us that there exists at least a dense subset of $\mathfrak{H}$; more generally, for a (not necessarily countable) but dense domain of the linear operator A, i.e. $\mathfrak{D}(A) \subseteq \mathfrak{H}$ and $\overline{\mathfrak{D}(A)} = \mathfrak{H}$, we can define its *adjoint* A^* as

$$A^* : \mathfrak{D}(A^*) \subseteq \mathfrak{H} \longrightarrow \mathfrak{H}$$
$$\psi \mapsto \theta$$

for a θ from[153]

$$\mathfrak{D}(A^*) := \{\psi \in \mathfrak{H} : \exists \theta \in \mathfrak{H} \text{ s.t. } \langle\psi, A\phi\rangle_{\mathfrak{H}} = \langle\theta, \phi\rangle_{\mathfrak{H}},\ \forall \phi \in \mathfrak{H}\};$$

we call A *self-adjoint*[154] if $A = A^*$ (i.e. their domains are identical and they agree on

[150] For more details about linear spaces, inner products, and other general notions such as the one of completeness, we invite the reader to skim through [Tes14, p.3-p.27].

[151] We abuse the notation by using '$\mathfrak{H}$' to refer to the whole Hilbert space, but the reader should have in mind $(\mathfrak{H}, +, \cdot, \langle\cdot,\cdot\rangle)$ whenever the context is appropriate.

[152] A separable space M is a topological space that has a countable proper subset $N \subsetneq M$ that is *dense*, i.e. its closure satisfies $\overline{N} = M$.

[153] The fact that $\mathfrak{D}(A)$ is dense in $\mathfrak{H}$ ensures that the mapping is well-defined [Tes14, p.68], by which we mean that θ is unique.

[154] Unfortunately, the fact that an operator A is satisfying the property $\langle A\cdot, \cdot\rangle = \langle\cdot, A\cdot\rangle$ (such an operator is called *Hermitian* in the physics literature, known in mathematics as *symmetric*) is not enough to develop the functional calculus we are aiming at in the latter part of the section, from which fundamental properties of the Schrödinger equation follow (see Corollary A.2.1); hence, in view of the importance of the functional calculus and its implications, it is justified to introduce a stronger definition for a self-adjoint operator.

every element of their identical domains).

The OQM observables are self-adjoint by definition (Axiom 1). In particular, the fact that we require the Hamiltonian H to be self-adjoint proves to be a sufficient condition to unlock the fundamental properties of the Hamiltonian evolution encoded in Corollary A.2.1, as we shall see shortly.

In Subsection 1.4, we motivated the introduction of the time-dependent Schrödinger equation on the basis of the time-independent Schrödinger equation

$$H\psi = E\psi, \tag{176}$$

and the plausible assumption that a state ψ satisfying (176) evolves in time according to

$$\psi(t) = e^{-itE}\psi = e^{-itH}\psi, \tag{177}$$

owing to the *Planck relation*

$$E = \omega.$$

We insisted that we need an equation that will allow for solutions of the type (177), so we came with (39). However, although the passage from (39) to $\psi(t)$ is trivial once we assume that (176) holds for $\psi := \psi(0)$, the state of affairs is totally different when ψ satisfies (39), but is **not** a solution of (176).

In the remaining part of appendix A, we will briefly explain how one can solve the time-dependent Schrödinger equation by exponentiation, or, in other words, how we can generalize (177) to arbitrary states $\psi \in \mathfrak{D}(H)$ (that are not necessarily eigenfunctions of the Hamiltonian).

To build some intuition for what lies ahead of us, we will start with a simple example from linear algebra: assume that the mapping $t \mapsto \psi(t)$ is an element of the continuously differentiable complex-valued functions defined on the real axis $C^1(\mathbb{R})$, and replace in (39) the Hamiltonian H with a constant matrix $M \in \mathbb{C}^{m\times m}$, such that we obtain

$$\frac{d\psi(t)}{dt} = -iM\psi(t)$$

i.e. a time-dependent Schrödinger-like equation, in mathematical jargon a matrix differential equation with constant matrix, with the solution given by

$$\psi(t) = e^{-itM}\psi,$$

for $\psi := \psi(0)$ and

$$e^{-itM} := \sum_{k=1}^{\infty} \frac{(-it)^k}{k!} M^k, \tag{178}$$

the matrix exponential. What did we use to define (178)? To avoid any ambiguity, let us recast it in a general way, i.e. what do we need to make sense of

$$e^M := \sum_{k=1}^{\infty} \frac{1}{k!} M^k \ ? \tag{179}$$

Common sense dictates that we must be certain that the defining infinite series converges in a norm appropriate to our goals, which we take as the induced matrix norm[155] (a particular case of the *operator norm*, see below)

$$\|M\|_{\mathrm{o}} := \sup_{v \in \mathbb{C}^m \setminus \{\mathbf{0}\}} \frac{\|Mv\|_{\mathbb{C}^m}}{\|v\|_{\mathbb{C}^m}}, \tag{180}$$

the $\|\cdot\|_{\mathbb{C}^m}$ above being the Euclidean norm in $\mathbb{C}^m$. Using (180) and the fact that $\|M^m\|_{\mathrm{o}} \leq \|M\|_{\mathrm{o}}^m$, the convergence of the defining infinite series for the matrix exponential is a standard proof. Likewise, we can take a step further in generality and define e^A for *bounded linear operators* A, i.e. the ones that satisfy

$$\|A\psi\|_{\mathfrak{H}} \leq C\|\psi\|_{\mathfrak{H}}, \text{ for all } \psi \in \mathfrak{D}(A) \setminus \{\mathbf{0}\}, \text{ and a fixed } C > 0; \tag{181}$$

the condition (181) is necessary and sufficient to define a more general[156] operator norm in exactly the same way as in (180), and similarly by using it we can show that the infinite series $\sum_{k=1}^{\infty}(1/k!)A^k$ converges (by exponentiation of A we mean self-composition).

However, for linear operators A that do not satisfy (181), which we will simply call *unbounded linear operators*, the supremum we used to define the operator norm fails to exist, so we cannot use the Taylor-like expansion (179) to 'create' the mathematical object 'e^A'. Why is it so? Because without the operator norm of A we cannot assess whether the aforementioned expansion convergences. We need a brand new route to get to a well-defined 'e^A', and along the way we hope to capture as many properties of the matrix exponential as is possible (the ones in [Hal13, p.340], for example), such that we can use it in applications.

Formally, the route to a well-defined and useful 'e^A' is encoded in the spectral theorem for self-adjoint operators[157], be they bounded or not:

[155] We are allowed to take the supremum (which in this context is achieved, so we can replace it with the maximum) over all $v \in \mathbb{C}^m \setminus \{\mathbf{0}\}$, as there is a $C > 0$ such that $\|Mv\|_{\mathbb{C}^m}/\|v\|_{\mathbb{C}^m} \leq C$ for any $v \in \mathbb{C}^m$ (as its domain $\mathfrak{D}(M) = \mathbb{C}^m$ is finite-dimensional, see [Kre89, p.96]).

[156] If, however, $\mathfrak{H}$ has finite dimension, then every linear operator is automatically bounded [Kre89, p.96].

[157] Which is a mathematical tour de force in its own right, therefore we redirect the reader to [RS80, Ch.VII-Ch.VIII].

Theorem A.1 (Spectral theorem for self-adjoint operators, the functional calculus form). *For $A : \mathfrak{D}(A) \subseteq \mathfrak{H} \longrightarrow \mathfrak{H}$ self-adjoint, there exists a unique mapping*

$$\Phi : \mathbb{B}^b_{\mathfrak{D}(A)} \longrightarrow L(\mathfrak{H}),$$

where

$$\mathbb{B}^b_{\mathfrak{D}(A)} = \{f : M_{\mathfrak{D}(A)} \subseteq \mathbb{R} \longrightarrow \mathbb{C} : f \text{ Borel measurable and bounded}\} \tag{182}$$

and as usual

$$L(\mathfrak{H}) = \left\{ F : \mathfrak{H} \longrightarrow \mathfrak{H} \text{ linear } : \sup_{\psi \in \mathfrak{H} \setminus \{\mathbf{0}\}} \frac{\|F\psi\|_{\mathfrak{H}}}{\|\psi\|_{\mathfrak{H}}} < \infty \right\},$$

with the properties

1. *For any f, $g \in \mathbb{B}^b_{\mathfrak{D}(A)}$ and $\lambda \in \mathbb{R}$, it is true that:*

$$\Phi(fg) = \Phi(f)\Phi(g), \quad \Phi(\lambda f) = \lambda \Phi(f),$$

$$\Phi\left(\mathbb{1}_{M_{\mathfrak{D}(A)}}\right) = \mathbb{I}, \quad \Phi(\overline{f}) = \Phi(f)^*.$$

2. $\|\Phi(f)\|_{L(\mathfrak{H})} \leq \|f\|_\infty$.

3. *Let $\{f_n\}_{n=1}^\infty \subseteq \mathbb{B}^b_{\mathfrak{D}(A)}$ be such that $f_n(x) \to x$ as $n \to \infty$, $\forall x \in M_{\mathfrak{D}(A)}$, and $|f_n(x)| \leq x$, $\forall x \in M_{\mathfrak{D}(A)}$ and $\forall n \in \mathbb{N}$. Then, for any $\psi \in \mathfrak{D}(A)$, we have that:*

$$\lim_{n\to\infty} \Phi(f_n)\psi = A\psi.$$

4. *If $\{f_n\}_{n=1}^\infty \subseteq \mathbb{B}^b_{\mathfrak{D}(A)}$ satisfies $f_n(x) \to f(x)$ for $\forall x \in M_{\mathfrak{D}(A)}$, and moreover $\exists R$ such that $\|f_n\|_\infty \leq R$, then*

$$\operatorname*{s-lim}_{n\to\infty} \Phi(f_n) = \Phi(f).$$

We call Φ the functional calculus.

We stress the fact that the domain[158] of the functions in (182) depends on $\mathfrak{D}(A)$, hence the notation '$M_{\mathfrak{D}(A)}$'. Now, for $H : \mathfrak{D}(H) \subseteq \mathfrak{H} \longrightarrow \mathfrak{H}$ self-adjoint, we introduce

$$f : M_{\mathfrak{D}(H)} \subseteq \mathbb{R} \longrightarrow \mathbb{C}$$

[158] In [RS80, Ch.VII-Ch.VIII] there are other versions of the same theorem, as well as the explicit expression for $M_{\mathfrak{D}(A)}$, which we omit here, as we strive to provide a brief sketch on how one can use the functional calculus defined in Theorem A.1.

via

$$x \mapsto e^{-itx},$$

and observe that it is easy to check that $f \in \mathbb{B}^b_{\mathfrak{D}(H)}$. Consequently, using Theorem A.1, we can define

$$e^{-itH} := \Phi(f),$$

and we expect

$$\psi(t) = e^{-itH}\psi(0) \tag{183}$$

to be equivalent to the time-dependent Schrödinger equation

$$\frac{d\psi(t)}{dt} = -iH\psi(t) \text{ with } \psi(0) = \psi. \tag{184}$$

The connection between (183) and (184) is, informally speaking, via

$$i\frac{d}{dt}e^{-itH} = He^{-itH}, \tag{185}$$

but what is the meaning of the derivative of e^{-itH}? We take a step back and take a closer look at Theorem A.1, to infer extra properties about e^{-itH}. Firstly, define

$$\lim_{t\to s} e^{-itH}\psi := \phi,$$

where $\phi \in \mathfrak{H}$ satisfies

$$\lim_{t\to s} \|e^{-itH}\psi - \phi\|_{\mathfrak{H}} = 0. \tag{186}$$

The equation (185) implies that we should have

$$\mathfrak{D}(H) = \left\{\psi \in \mathfrak{H} : t \mapsto e^{-itH}\psi \text{ is differentiable}\right\},$$

by which we mean, using (186) as our definition of a limit, that

$$\mathfrak{D}(H) = \left\{\psi \in \mathfrak{H} : \exists \phi \in \mathfrak{H} \text{ s.t. } \forall s \in \mathbb{R} \lim_{t\to s} \left\| \frac{e^{-itH}\psi - e^{-isH}\psi}{t} - \phi \right\|_{\mathfrak{H}} = 0\right\}. \tag{187}$$

The domain above is an extra requirement on the self-adjoint operator H, or so it seems at a first glance. However, it can be proven [DT09, p.332] that if $H = H^*$, then the latter is the *generator* of $\{e^{-itH}\}_{t\in\mathbb{R}}$, i.e. it satisfies the extra condition (187) automatically, and further

$$i\frac{d}{dt}e^{-itH}\psi = He^{-itH}\psi,$$

for any $\psi \in \mathfrak{D}(H)$, thus answering to (185) (the converse of this fact goes by the name of Stone's theorem [Tes14, p.147]). It then follows from the spectral theorem for self-adjoint operators that:

Lemma A.2. *If H is self-adjoint, then the family of operators $\{e^{-itH}\}_{t\in\mathbb{R}}$, defined using Theorem A.1, forms a group with the operation of map composition. Moreover, we have the properties:*

1. *$t \mapsto e^{-itH}\psi$ is strongly continuous for any $\psi \in \mathfrak{H}$, i.e.*

$$\lim_{t\to s} \|e^{-itH}\psi - e^{-isH}\psi\|_{\mathfrak{H}} = 0,$$

   for an arbitrary $s \in \mathbb{R}$.

2. *$e^{-i(t+s)H} = e^{-itH}e^{-isH}$, for any t, $s \in \mathbb{R}$.*

3. *$e^{-i0H} = \mathbb{I}$.*

4. *$\|e^{-itH}\psi\|_{\mathfrak{H}} = \|\psi\|_{\mathfrak{H}}$, for any $\psi \in \mathfrak{H}$ and $t \in \mathbb{R}$.*

In light of the properties afferent to Lemma A.2, we can say that $\{e^{-itH}\}_{t\in\mathbb{R}}$ with map composition is a *strongly continuous unitary group*. Indeed, the *isometricity* of e^{-itH}, i.e. property 4 of Lemma A.2, takes care that $\psi(t)$ is normalized, a condition necessary for it to be a state, as discussed in Axiom 1, and also it confirms the calculation done in (40). Moreover, Lemma A.2 provides us with the existence of $\psi(t)$ at all times, as well as the following fundamental properties

Corollary A.2.1. *With $H = H^*$ and $\psi \in \mathfrak{D}(H)$, we have*

1. *Uniqueness of solutions, by which we mean $e^{-itH}\psi_1 = e^{-itH}\psi_2 \iff \psi_1 = \psi_2$.*

2. *Commutativity, i.e. $e^{-itH}H\psi = He^{-itH}\psi$.*

3. *Invariance, in the sense that $e^{-itH}\psi \in \mathfrak{D}(H)$, for any $t \in \mathbb{R}$.*

To recapitulate, in this part of the appendix we showed that the time-dependent Schrödinger equation can be reformulated as

$$\psi(t) = e^{-itH}\psi(0),$$

with e^{-itH} defined using the functional calculus introduced in Theorem A.1. This approach brings rigour to many of the calculations we did as part of Section 1, an example being (40).

B. Kato's criterion for self-adjointness of the Hamiltonian

First and foremost, choosing a potential V should be done in such a way that H turns out to be self-adjoint, as specified by Axiom 2 in Section 1. Fortunately, Kato [Kat51] proved the general fact[159] that for

$$V : \mathbb{R}^m \longrightarrow \mathbb{R} \tag{188}$$

that can be written as

$$V(\mathbf{x}) = V_1(\mathbf{x}) + V_2(\mathbf{x}), \tag{189}$$

and for which the requirements

$$\begin{aligned} &|V_1(\mathbf{x})| < \infty, \ \forall \mathbf{x} \in \mathbb{R}^m \\ &\int_\Upsilon |V_2(\mathbf{x})|^2 \, d^m x < \infty, \quad \forall \Upsilon \subsetneq \mathbb{R}^m \text{ compact} \\ &\lim_{x_i \to \pm\infty} V_2(\mathbf{x}) < \infty, \ \forall i \in \{1, ..., m\} \end{aligned} \tag{190}$$

are met, we have that H is self-adjoint and $\mathfrak{D}(H) = \mathfrak{D}(H_0)$ (the three requirements in (190) are called boundedness of V_1, and local square integrability, boundedness at infinity of V_2, respectively).

As many physically relevant potentials are (modulo multiplication by a constant) of the shape $V(\mathbf{x}) = |\mathbf{x}|^a$, $a \in \mathbb{R}$, plugging the latter[160] in (190), we obtain that boundedness of V_1 is satisfied for any $a \in \mathbb{R}$, as $V_1(\mathbf{x}) = 0$ in this case, that local square integrability of V_2 imposes[161] that $a > -m/2$, while boundedness at infinity of V_2 mandates $a \leq 0$; intersecting these three conditions, we get that $a \in (-m/2, 0]$ is a sufficient condition for choosing a potential of the specified form such that H is self-adjoint and $\mathfrak{D}(H) = \mathfrak{D}(H_0)$. In particular, in the case of the Coulomb potentials, for which $a = -1$, we know for sure from the result presented above that if the dimension of the 'physical space' is $m > 2$, then it is certain that H will behave as we expect from more heuristic treatments of quantum mechanics; however, in the case $m = 1$ and $m = 2$, Kato's criterion for

[159] The straightforward generalization to an arbitrary number of particles is also true, but it makes further assumptions on the form of V, i.e. it requires V to be expressible as a sum of a bounded function in the whole configuration space and terms that are not dependent on all the configuration space.

[160] For the sake of rigour, we remark that for $a < 0$ we have an infinite discontinuity on the singleton $\{\mathbf{x} = 0\}$, which is obviously of Lebesgue measure zero.

[161] We found it convenient to express V_2 in spherical coordinates in $\mathbb{R}^m$, and to observe that in this case square integrability over Υ compact and arbitrary is equivalent to square integrability over B_R, for any arbitrary $R > 0$.

self-adjointness becomes uninformative (fortunately, there are no problems with the case $m = 3$, the dimension that corresponds to real-world experiments in a nonrelativistic setting).

Theorem B.1 (Kato's criterion for self-adjointness of H)**.** *For a potential (188) that can be decomposed in two parts as in (189) and satisfies boundedness, local integrability, and boundedness at infinity of its respective parts (190), we have that* $H = H^*$ *and* $\mathfrak{D}(H) = \mathfrak{D}(H_0)$*. In particular, for potentials of the form* $V(\mathbf{x}) = |\mathbf{x}|^a$*, it is sufficient to take* $a \in (-m/2, 0]$.

C. Spread of the free wave function

Lemma C.1 (Spread of the free wave function)**.** *For $\psi \in L^1(\mathbb{R}^m) \cap L^2(\mathbb{R}^m)$ and $t \neq 0$, the following inequality holds true*

$$\|e^{-itH_0}\psi\|_\infty \leq |4\pi t|^{-m/2}\|\psi\|_{L^1}. \tag{191}$$

Proof. As it is explained in [Tes14, p.199-p.200], the free propagator e^{-itH_0} is diagonalized by the Fourier transform $\mathcal{F}$

$$e^{-itH_0}\psi(\mathbf{x}) = \mathcal{F}^{-1}e^{-it|\mathbf{x}|^2}(\mathcal{F}\psi)(\mathbf{x}), \tag{192}$$

hence it follows that the argument in the sup norm on the left-hand side of (191) can be represented as

$$e^{-itH_0}\psi(\mathbf{x}) = (4\pi it)^{-m/2}\int_{\mathbb{R}^m} e^{i|\mathbf{x}-\mathbf{y}|^2/4t}\psi(\mathbf{y})\, d^m y, \tag{193}$$

so

$$\begin{aligned}|e^{-itH_0}\psi(\mathbf{x})| \leq& |4\pi it|^{-m/2}\int_{\mathbb{R}^m} |e^{i|\mathbf{x}-\mathbf{y}|^2/4t}\psi(\mathbf{y})|\, d^m y\\ =&|4\pi t|^{-m/2}\int_{\mathbb{R}^m} |\psi(\mathbf{y})|\; d^m y\\ =&|4\pi t|^{-m/2}\|\psi\|_{L^1} < \infty,\end{aligned} \tag{194}$$

because ψ is integrable, and as the complex magnitude of the free particle evolution is bounded from above via (194) for any $\mathbf{x} \in \mathbb{R}^m$, we can take the supremum over all the $\mathbf{x} \in \mathbb{R}^m$ to conclude that (191) is true. □

Although ψ was chosen in Lemma C.1 with the extra requirement of being integrable on $\mathbb{R}^m$, it is nevertheless interesting to investigate the dynamical consequences of (191): we simply square it to obtain

$$\rho(\mathbf{x}, t) := |e^{-itH_0}\psi(\mathbf{x}, t)|^2 \leq \|e^{-itH_0}\psi\|_\infty^2 \leq |4\pi t|^{-m}\|\psi\|_{L^1}^2 \propto t^{-m}, \tag{195}$$

i.e. it implies that the probability density function ρ at any point of space $\mathbf{x} \in \mathbb{R}^m$ and time $t \geq 1$ is bounded from above by a decreasing function $\propto t^{-m}$.

However, as

$$\int_{\mathbb{R}^m} \rho(\mathbf{x})\, d^m x = \|e^{-itH_0}\psi\|^2 = 1, \quad \forall t \in \mathbb{R},$$

as the particle has to be somewhere, the only choice left for the probability density function ρ is ‘to spread’.

Moreover, under the free evolution, we expect that a particle will asymptotically leave any Borel measurable bounded[162] subset $\Upsilon \subseteq \mathbb{R}^m$ almost surely, as from (195) with $\ddot{c} := |4\pi t|^{-m}\|\psi\|_{L^1}^2$ we can further infer that

$$\begin{aligned} P_t^{\mathrm{OQM}}(\Upsilon) &= \int_{\Upsilon} |e^{-itH_0}\psi(\mathbf{x})|^2 \, d^m x \\ &\leq \ddot{c}\lambda(\Upsilon)t^{-m} \\ &\propto t^{-m}, \end{aligned}$$

a situation which agrees with our physical intuition.

[162]The Lebesgue measure λ is finite on bounded sets of $\mathbb{R}^m$.

D. Technical lemmas

In here we collect all the lemmas that were not relevant enough from a mathematical/physical point of view to make it to the main text of the thesis. All the same, some of them are derived using interesting properties, and can even give us a rough idea about the physics they refer to.

Lemma D.1 (The factorization of the free evolution)**.** *For $t \neq 0$, the free evolution admits the factorization into unitary operators*

$$e^{-itH_0} = C_t Q_t, \tag{196}$$

where Q_t is

$$\psi(\mathbf{x}) \mapsto e^{i|\mathbf{x}|^2/4t}\psi(\mathbf{x}), \tag{197}$$

and C_t is

$$\psi(\mathbf{x}) \mapsto (2it)^{-m/2} e^{i|\mathbf{x}|^2/4t}(\mathcal{F}\psi)(\mathbf{x}/2t), \tag{198}$$

both defined pointwisely for an $\mathbf{x} \in \mathbb{R}^m$, with a $\psi \in L^2(\mathbb{R}^m)$.

Proof. Calculating

$$\|Q_t\psi\|^2 = \int_{\mathbb{R}^m} |e^{i|\mathbf{x}|^2/4t}\psi(\mathbf{x})|^2 \, d^m x = \int_{\mathbb{R}^m} |\psi(\mathbf{x})|^2 \, d^m x = \|\psi\|^2, \tag{199}$$

$$\|C_t\psi\|^2 = |2t|^{-m} \int_{\mathbb{R}^m} |(\mathcal{F}\psi)(\mathbf{x}/2t)|^2 \, d^m x = \int_{\mathbb{R}^m} |\psi(\mathbf{k})|^2 \, d^m k = \|\mathcal{F}\psi\|^2 = \|\psi\|^2, \tag{200}$$

we see that they are isometries[163], hence automatically continuous and injective, and surjectivity comes in the case of (197) simply from the fact that for any $\psi \in \mathfrak{R}(Q_t)$, the pointwisely defined square-integrable $e^{-i|\mathbf{x}|^2/4t}\psi(\mathbf{x})$ is the corresponding element of $\mathfrak{D}(Q_t) = L^2(\mathbb{R}^m)$, while for (198) we additionaly note that $\mathcal{F}$ extended to all $L^2(\mathbb{R}^m)$ is still bijective, and then the rest of the argument follows similarly. Thus C_t and Q_t are unitary.

The continuity of the operators provides us with some flexibility, as we need then to prove (196) only for a dense subset of $L^2(\mathbb{R}^m)$; as $\mathcal{F}$ appears in (198), the Schwartz space $S(\mathbb{R}^m)$ is a natural choice to continue the proof.

The Schwartz space $S(\mathbb{R}^m)$ is defined as

$$S(\mathbb{R}^m) := \left\{ f \in C^\infty(\mathbb{R}^m) : \sup_{\mathbf{x}\in\mathbb{R}^m} |\mathbf{x}^{\boldsymbol{\alpha}} \partial_{\boldsymbol{\beta}} f(\mathbf{x})| < \infty, \text{ for all } \boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}_0^m \right\}, \tag{201}$$

[163] We also used the fact that $\mathcal{F}$ is an isometry on $L^2(\mathbb{R}^m)$ for the fourth equality in (200).

with

$$\mathbf{x}^{\boldsymbol{\alpha}} \coloneqq \prod_{i=1}^{m} x_i^{\alpha_i}, \quad \partial_{\boldsymbol{\beta}} f \coloneqq \frac{\partial^{|\boldsymbol{\beta}|} f}{\partial^{\beta_1} x_1 \ldots \partial^{\beta_m} x_m},$$

for $\boldsymbol{\alpha} \coloneqq (\alpha_1, \ldots, \alpha_m)$, $\boldsymbol{\beta} \coloneqq (\beta_1, \ldots, \beta_m)$ and $|\boldsymbol{\beta}| \coloneqq \sum_{i=1}^{m} \beta_m$ (additionally, we also set $(\lambda \mathbf{x})^{\boldsymbol{\alpha}} \coloneqq \lambda^{|\boldsymbol{\alpha}|} \mathbf{x}^{\boldsymbol{\alpha}}$ for a $\lambda \in \mathbb{R}$). We have that $S(\mathbb{R}^m)$ is a dense linear subspace of $L^p(\mathbb{R}^m)$ for $p \in [1, \infty)$, and also $\mathcal{F}S(\mathbb{R}^m) \subseteq S(\mathbb{R}^m)$ [Tes14, p.187].

To continue our proof, take $\psi \in S(\mathbb{R}^m)$ arbitrary. We use (197) and (198) to obtain

$$(C_t Q_t f)(\mathbf{x}) = (2it)^{-m/2} e^{i|\mathbf{x}|^2/4t} (\mathcal{F} Q_t \psi)\left(\mathbf{x}/2t\right), \tag{202}$$

where

$$(\mathcal{F} Q_t \psi)\left(\mathbf{x}/2t\right) = (2\pi)^{-m/2} \int_{\mathbb{R}^m} e^{i(|\mathbf{y}|^2/4t - \mathbf{x}\cdot\mathbf{y}/2t)} \psi(y)\, d^m y. \tag{203}$$

Consequently, combining (202) with (203), we get

$$\begin{aligned}
(C_t Q_t f)(\mathbf{x}) =& (2it)^{-m/2} e^{i|\mathbf{x}|^2/4t} (2\pi)^{-m/2} \int_{\mathbb{R}^m} e^{i(|\mathbf{y}|^2/4t - \mathbf{x}\cdot\mathbf{y}/2t)} \psi(\mathbf{y})\, d^m y \\
=& (4\pi i t)^{-m/2} \int_{\mathbb{R}^m} e^{i(|\mathbf{y}|^2/4t - \mathbf{x}\cdot\mathbf{y}/2t + |\mathbf{x}|^2/4t)} \psi(\mathbf{y})\, d^m y \\
=& (4\pi i t)^{-m/2} \int_{\mathbb{R}^m} e^{i|\mathbf{x}-\mathbf{y}|^2/4t} \psi(\mathbf{y})\, d^m y,
\end{aligned}$$

which agrees with (193) over $S(\mathbb{R}^m)$. □

Lemma D.2. *For any $\psi \in L^2(\mathbb{R}^m)$ and $t \neq 0$, it holds true that*

$$\lim_{t\to\pm\infty} \|e^{-itH_0}\psi - C_t \psi\| = 0 \tag{204}$$

Proof. Using Lemma D.1, one may compute

$$\begin{aligned}
\|e^{-itH_0}\psi - C_t\psi\|^2 =& \|C_t Q_t \psi - C_t \psi\|^2 = \|C_t(Q_t\psi - \psi)\|^2 = \|Q_t\psi - \psi\|^2 \\
=& \int_{\mathbb{R}^m} |e^{i|\mathbf{x}|^2/4t} - 1|^2 |\psi(\mathbf{x})|^2\, d^m x,
\end{aligned}$$

and as $|e^{i|\mathbf{x}|^2/4t} - 1|^2 |\psi(\mathbf{x})|^2 = (2 - 2\cos(|\mathbf{x}|^2/4t))|\psi(\mathbf{x})|^2 \to 0$ as $t \to \pm\infty$, and moreover noticing that $|e^{i|\mathbf{x}|^2/4t} - 1|^2 |\psi(\mathbf{x})|^2 \leq 4|\psi(\mathbf{x})|^2$, the latter being integrable by assumption, Lebesgue's dominated convergence theorem implies (204). □

Lemma D.3. *Let $\psi_1(t)$, $\psi_2(t) \in L^2(\mathbb{R}^m)$, $\forall t \in \mathbb{R}$, and take the mappings $t \mapsto \psi_1(t)$, $t \mapsto \psi_2(t)$ to be continuous. Moreover, assume further that $\|\psi_1(t)\| = \|\psi_2(t)\| = 1$, that*

$$\lim_{t\to\pm\infty} \|\psi_1(t) - \psi_2(t)\| = 0,$$

and that $\Upsilon \subseteq \mathbb{R}^m$ is a Borel measurable set. Then we have that

$$\lim_{t\to\pm\infty} \int_{\Upsilon} |\psi_1(t,\mathbf{x})|^2\, d^m x \text{ exists iff } \lim_{t\to\pm\infty} \int_{\Upsilon} |\psi_2(t,\mathbf{x})|^2\, d^m x \text{ exists,} \tag{205}$$

and consequently if the limits in (205) do exist, then they are equal.

Proof. Take $\psi_1(t),\ \psi_2(t) \in L^2(\mathbb{R}^m)$ with the above properties so that

$$
\begin{aligned}
0 \leq & \left| \int_\Upsilon \left\{ |\psi_1(t,\mathbf{x})|^2 - |\psi_2(t,\mathbf{x})|^2 \right\} d^m x \right| \\
\leq & \int_\Upsilon \left| |\psi_1(t,\mathbf{x})|^2 - |\psi_2(t,\mathbf{x})|^2 \right| d^m x \\
\leq & \int_{\mathbb{R}^m} \left| |\psi_1(t,\mathbf{x})|^2 - |\psi_2(t,\mathbf{x})|^2 \right| d^m x \\
= & \int_{\mathbb{R}^m} \Big(|\psi_1(t,\mathbf{x})| - |\psi_2(t,\mathbf{x})| \Big) \Big(|\psi_1(t,\mathbf{x})| + |\psi_2(t,\mathbf{x})| \Big) d^m x \\
\leq & \Big\| |\psi_1(t)| + |\psi_2(t)| \Big\| \; \Big\| \psi_1(t) - \psi_2(t) \Big\| \\
\leq & \Big(\|\psi_1(t)\| + \|\psi_2(t)\| \Big) \|\psi_1(t) - \psi_2(t)\| \\
= & 2 \|\psi_1(t) - \psi_2(t)\|,
\end{aligned}
\tag{206}
$$

which was obtained using standard methods, i.e. the (inverse) triangle and Cauchy-Schwartz inequality. As $\lim_{t\to\pm\infty} \|\psi_1(t) - \psi_2(t)\| = 0$, the squeeze theorem applied to the estimates in (206) leads to

$$
\lim_{t\to\pm\infty} \left\{ \int_\Upsilon |\psi_1(t,\mathbf{x})|^2 \, d^m x - \int_\Upsilon |\psi_2(t,\mathbf{x})|^2 \, d^m x \right\} = 0, \tag{207}
$$

so by defining

$$
\Lambda(t) := \int_\Upsilon |\psi_1(t,\mathbf{x})|^2 \, d^m x - \int_\Upsilon |\psi_2(t,\mathbf{x})|^2 \, d^m x,
$$

and by assuming without loss of generality that

$$
\exists \lim_{t\to\pm\infty} \int_\Upsilon |\psi_1(t,\mathbf{x})|^2 \, d^m x,
$$

then by expressing the other as

$$
\int_\Upsilon |\psi_2(t,\mathbf{x})|^2 \, d^m x = \left\{ \int_\Upsilon |\psi_1(t,\mathbf{x})|^2 \, d^m x - \Lambda(t) \right\}, \tag{208}
$$

it follows that the function on the right-hand side is a sum of two functions who have a limit at $t \to \pm\infty$, hence itself has a limit. Lastly, by (207) applied to (208) as $t \to \pm\infty$, we obtain the identity

$$
\lim_{t\to\infty} \int_\Upsilon |\psi_2(t,\mathbf{x})|^2 \, d^m x = \lim_{t\to\infty} \int_\Upsilon |\psi_1(t,\mathbf{x})|^2 \, d^m x.
$$

$\square$

References

[AAV88] Y. Aharonov, D. Z. Albert, and L. Vaidman. How the result of a measurement of a component of the spin of a spin-1/2 particle can turn out to be 100. *Physical review letters*, 60 14:1351–1354, 1988.

[ACE14] Y. Aharonov, E. Cohen, and A. Elitzur. Foundations and Applications Of Weak Quantum Measurements. *Physical Review A*, 89:052105, 2014.

[AdP06] P. Atkins and J. de Paula. *Physical Chemistry for the Life Sciences*. Oxford University Press, 2006.

[ADR82] A. Aspect, J. Dalibard, and G. Roger. Experimental Test of Bell's Inequalities Using Time- Varying Analyzers. *Physical Review Letters*, 49(25):1804–1807, December 1982.

[BD04] P. Blanchard and G. Dell'Antonio. Multiscale Methods in Quantum Mechanics : Theory and Experiment. 2004.

[BDG+95] K. Berndl, D. Dürr, S. Goldstein, G. Peruzzi, and N. Zanghí. On the global existence of Bohmian mechanics. *Communications in Mathematical Physics*, 173:647–673, 1995.

[Bel64] J. S. Bell. On the Einstein Podolsky Rosen paradox. *Physics Physique Fizika*, 1(3):195–200, November 1964.

[Bel81] J. S. Bell. BERTLMANN'S SOCKS AND THE NATURE OF REALITY. *Le Journal de Physique Colloques*, 42(C2):C2–41–C2–62, March 1981.

[Boh35] N. Bohr. Can Quantum-Mechanical Description of Physical Reality Be Considered Complete? *Physical Review*, 48:696–702, July 1935.

[Boh52] D. Bohm. A Suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables. I. *Physical Review*, page 166–179, 1952.

[Bro27] L. Broglie. La mécanique ondulatoire et la structure atomique de la matière et du rayonnement. *Journal De Physique Et Le Radium*, 8:225–241, 1927.

[Coo57] J. M. Cook. Convergence to the Møller Wave-Matrix. *Journal of Mathematics and Physics*, 36:82–87, 1957.

[Dau95] M. Daumer. *Streutheorie aus der Sicht Bohmscher Mechanik*. PhD thesis, 1995. Fakultät für Mathematik und Informatik der Ludwig-Maximilians-Universität München.

[DDGZ95a] M. Daumer, D. Duerr, S. Goldstein, and N. Zanghí. On the quantum probability flux through surfaces. *arXiv: Quantum Physics*, 1995.

[DDGZ95b] M. Daumer, D. Dürr, S. Goldstein, and N. Zanghí. On the flux-across-surfaces theorem. *Letters in Mathematical Physics*, 38:103–116, 1995.

[DGN+14] D. Dürr, S. Goldstein, T. Norsen, W. Struyve, and N. Zanghí. Can bohmian mechanics be made relativistic? *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 470, 2014.

[DGZ92] D. Dürr, S. Goldstein, and N. Zanghí. Quantum equilibrium and the origin of absolute uncertainty. *Journal of Statistical Physics*, 67:843–907, 1992.

[DGZ96] D. Dürr, S. Goldstein, and N. Zanghí. Bohmian mechanics as the foundation of quantum mechanics. *arXiv: Quantum Physics*, pages 21–44, 1996.

[Dol64] J. D. Dollard. Asymptotic Convergence and the Coulomb Interaction. *Journal of Mathematical Physics*, 5:729–738, 1964.

[Dol69] J. D. Dollard. Scattering into Cones I: Potential Scattering. *Commun. math. Phys*, 12:193–203, 1969.

[DT00] D. Dürr and S. Teufel. On the role of flux in scattering theory. *Canadian Mathematical Society: Conference Proceedings*, 28, 2000.

[DT09] D. Dürr and S. Teufel. *Bohmian mechanics: the physics and mathematics of quantum theory.* Springer, Berlin ; London, 2009.

[Ens78] V. Enss. Asymptotic completeness for quantum mechanical potential scattering. *Communications in Mathematical Physics*, 61:285–291, 1978.

[EPR35] A. Einstein, B. Podolsky, and N. Rosen. Can Quantum-Mechanical Description of Physical Reality Be Considered Complete? *Physical Review*, 47(10):777–780, May 1935.

[Eve57] H. Everett. "Relative State" Formulation of Quantum Mechanics. *Reviews of Modern Physics*, 29:454–462, 1957.

[FC72] S. J. Freedman and J. F. Clauser. Experimental Test of Local Hidden-Variable Theories. *Physical Review Letters*, 28(14):938–941, April 1972.

[FGZ+19] Y. Y. Fein, P. Geyer, P. Zwick, F. Kiałka, S. Pedalino, M. Mayor, S. Gerlich, and M. Arndt. Quantum superposition of molecules beyond 25 kDa. *Nature Physics*, 15(12):1242–1245, December 2019.

[FM06] A. Fasano and S. Marmi. *Analytical Mechanics.* Oxford University Press, 2006.

[GRW86] G. C. Ghirardi, A. Rimini, and T. Weber. Unified dynamics for microscopic and macroscopic systems. *Physical review. D, Particles and fields*, 34 2:470–491, 1986.

[GS22] W. Gerlach and O. Stern. Der experimentelle Nachweis der Richtungsquantelung im Magnetfeld. *Zeitschrift für Physik*, 9(1):349–352, December 1922.

[GS07] S. Goldstein and W. Struyve. On the Uniqueness of Quantum Equilibrium in Bohmian Mechanics. *Journal of Statistical Physics*, 128:1197–1209, 2007.

[GTZ09] S. Goldstein, R. Tumulka, and N. Zanghí. Bohmian Trajectories as the Foundation of Quantum Mechanics. *arXiv: Quantum Physics*, 2009.

[Hal13] B. C. Hall. *Quantum Theory for Mathematicians.* Springer Science+Business Media, 2013. Graduate text in Mathematics.

[His12] P. Hislop. Fundamentals of scattering theory and resonances in quantum mechanics. 2012.

[Kat51] T. Kato. Fundamental properties of Hamiltonian operators of Schrödinger type. *Transactions of the American Mathematical Society*, 70:195–211, 1951.

[KBR+11] S. Kocsis, B. Braverman, S. Ravets, M. Stevens, R. Mirin, L. Shalm, and A. Steinberg. Observing the average trajectories of single photons in a two-slit interferometer. *Science*, 332:1170 – 1173, 2011.

[KK59] T. Kato and S. Kuroda. A remark on the unitarity property of the scattering operator. *Il Nuovo Cimento (1955-1965)*, 14:1102–1107, 1959.

[Kre89] E. Kreyszig. *Introductory Functional Analysis With Applications.* 1989.

[Kuh96] T. S. Kuhn. *The structure of scientific revolutions.* University of Chicago Press, Chicago, IL, 3rd ed edition, 1996.

[Lan93] S. Lang. *Real and Functional Analysis.* Springer-Varlag New York, 1993.

[Mau95] T. Maudlin. Why Bohm's Theory Solves the Measurement Problem. *Philosophy of Science*, 62:479 – 483, 1995.

[Omn94] R. Omnès. *The Interpretation of Quantum Mechanics.* Princeton University Press, 1994.

[RDM05] S. Roemer, D. Duerr, and T. Moser. Asymptotic behaviour of Bohmian trajectories in scattering situations. *Journal of Physics A*, 38:8421–8443, 2005.

[Rov21] C. Rovelli. Preparation in Bohmian Mechanics. 2021. https://arxiv.org/pdf/2104.11339.pdf.

[RS79] M. Reed and B. Simon. *Methods of Modern Mathematical Physics III: Scattering Theory.* Academic Press, INC., 1979.

[RS80] M. Reed and B. Simon. *Methods of Modern Mathematical Physics I: Functional Analysis.* Academic Press, INC., 1980. Revised and enlarged edition.

[Rud87] W. Rudin. *Real and Complex Analysis.* McGraw-Hill Book Company, third edition, 1987. International Edition.

[Rue69] D. Ruelle. A remark on bound states in potential-scattering theory. *Il Nuovo Cimento A (1965-1970)*, 61:655–662, 1969.

[Sch06] R. Schneider. Integral geometry – measure theoretic approach and stochastic applications. 2006.

[SKZ13] M. Schlosshauer, J. Kofler, and A. Zeilinger. A snapshot of foundational attitudes toward quantum mechanics. *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics*, 44(3):222–230, August 2013.

[SN11] J. J. Sakurai and J. Napolitano. *Modern quantum mechanics.* Addison-Wesley, Boston, 2nd ed edition, 2011.

[Tes14] G. Teschl. *Mathematical Methods in Quantum Mechanics with Applications to Schrödinger Operators*, volume 157. American Mathematical Society, second edition, 2014. Graduate Studies in Mathematics.

[Teu99] S. Teufel. *The flux-across-surfaces theorem and its implications for scattering theory.* PhD thesis, 1999. Fakultät für Mathematik und Informatik der Ludwig-Maximilians-Universität München.

[tH16] G. 't Hooft. *The cellular automaton interpretation of quantum mechanics.* Number 6001 in Fundamental theories of physics. Springer Berlin Heidelberg, New York, NY, 2016.

[Tum18] R. Tumulka. On Bohmian Mechanics, Particle Creation, and Relativistic Space-Time: Happy 100th Birthday, David Bohm! *Entropy*, 20, 2018.

[WA97a] D.B. Pearson W.O. Amrein. Flux and scattering into cones for long range and singular potentials. *Journal of Physics A*, 30, 1997.

[WA97b] J.L. Zuleta W.O. Amrein. Flux and scattering into cones in potential scattering. *Helv. Phys. Acta*, 70, 1997.

[Wer13] C. Werndl. Justifying Typicality Measures of Boltzmannian Statistical Mechanics and Dynamical Systems. *arXiv: History and Philosophy of Physics*, 2013.

[Yeh06] J. Yeh. *Real Analysis: Theory of Measure and Integration*. 2006.