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Time in Quantum Mechanics and Aspects of the Time-of-Arrival Problem

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Submitted on September 22th 2014 in partial fulfilment of the requirements for the degree of Master of Science of Imperial College London

Abstract

Time in Quantum Mechanics as a concept and as a measurable quantity is the general topic discussed inside this MSc Dissertation. The inherit difficulty of expressing formally the probabilistic expectation of time measurements via the standard procedure in Quantum Mechanics is explained, focusing specifically on the much studied time-of-arrival problem. Due weight is given in the perception of time measurements in the classical limit and in deriving for reference necessary classical statistical expressions for the time-of-arrival problem. The so called "Pauli's Theorem" is also explained in detail. While the main focus of the project is on the extensive and detailed presentation of two specific and highly disputable attempts by researchers to construct an apparatus-independent expression for the probability distribution of the time-of-arrival measurements for the free particle case using indeed self-adjoint expressions of operators, an option supposedly prohibited by the "Pauli's Theorem".

Contents

Chapter 1

Introduction

"... the time of transitions or 'quantum jumps' must be as concrete and determinable as, say, energies in stationary states."

— Werner Heisenberg (1927) [21]

It's again one of these cases in Physics where a problem so easily explained and defined can exhibit such an elusive tendency for a definite answer. Time in Quantum Mechanics. Time of arrival of particle, the time that it needs to reach to a specific point in space. What can possibly be difficult to express on these concepts? Don't we simply have to treat time like we do with space dimensions, "on the same footing" as we usually say for the spacetime concept of the (relativistic) quantum field theories?

The answer to the latter cannot be more ambiguous and the answer to the former cannot be anything else than discouraging. The perception of time in Quantum Mechanics has been a conceptual struggle for almost a hundred of years, leading to a cornucopia of ideas and methods in dealing with it and it has been since then a constant opportunity for contemplation again and again on the very foundations of the Quantum Mechanics.

1.1 So, what's wrong with time in Quantum Mechanics?

Our difficulty with the perception of time in Quantum Mechanics, or the quantization of time, mustn't be misunderstood as some bizarre and scholastic obsession for a consistent philosophical definition of time in the quantum level. Actually, we don't even suppose much difference with the Newtonian time in Quantum Mechanics, since it is assumed that we are safely away from the relativistic limit. As mentioned above, the inaugural question for the problem that we're dealing with on the concept of time, of time intervals, in Quantum Mechanics, is easily posed and initially quite easy to be understood. It's the typical question, as in Classical Mechanics, of *"when"* a well-defined incident is about to happen.

In Classical Physics, despite of any definitions we would like to assign to the concept of time, this specific question is first of all and clearly a question on measurement; time measurement with devices (clocks) or without (from direct calculation of time intervals from other measurable parameters). Time as measurement is both a parameter inside our equations and an index on our (very accurate nowadays) clocks. And we can arrange for these two definitions to coincide very precisely.

Naturally so, this was the kind of questions that were primarily posed by the pioneers of Quantum Mechanics when they were contemplating on these very bizarre and mysterious phenomena for them, the famous "quantum jumps": *"when"* an atomic electron will change its state from a higher-energy state to a one of lower energy, for the emission of a photon?, they wondered [29]. This kind of reflections maybe seem naïve for us on hindsight, but they deserve more appreciation since still, almost a hundred years after they were conceived, there's not a definite answer. They evolved tough in more recent years to much more sophisticated questions, like: "When does a Measurement or Event Occur?" [30], where the concept of "event" tries to enter the quantum realm, calling for a change on the fundamental postulates of the Quantum Mechanics [6].

And again this absence of a definite answer is not because of any technical or computational reasons, not even because of experimental data discrepancies. On the contrary, experimentalists perform measurements of time quantities, *time-of-flight* measurements, *tunnelling times*, decay rates etc, in a daily routine, in any degree of accuracy desired, at impressive small scales, reaching nowadays to the, unimaginable even for some decades ago, level of one-particle experiments.

So what's the exact difficulty concerning measurements of time intervals in Quantum Mechanics? Quantum Mechanics inherently admits a probabilistic character for any kind of measurement procedures and hence a measurement of time too in the quantum level is expected to follow this characteristic. More accurately then, the question on "when" must be rephrased to: "when" is expected for something to happen?, demanding an answer of probabilistic nature.

Since then Quantum Mechanics as a system has managed, through the experience of so many years, to successfully formulate mathematically this probabilistic character for measurements of various other quantities, a corresponding expression for time measurements wasn't expected to exhibit any particular difficulty in obtaining it. Time was already a dynamical parameter [32] inside our mathematical expressions of states and amplitudes through one of the most important equation of Quantum Mechanics, the Schrödinger equation. And on the other hand, generations of experimentalists manage to give us progressively even more accurate expectations values on time quantities on various phenomena, from *lifetimes* to *dwell times*. There must be a link between these two; we must be able to write down on paper an accurate probability distribution on when a particle radiated from source will be detected. Or we simply cannot do it? There are indeed researchers suggest our inherit incapability in doing so.

This question still remains for the simple reason that we couldn't manage to decide yet if the time measurements we conduct, even for the simplest ones, are dependent on the apparatus used for this purpose or not. And this is definitely not something we can easily go along with. A measurement in Quantum Mechanics indeed is a destructive procedure; after the measurement of a quantity performed on a system, no other information is available to be known for this system for the simple reason that the system has changed due to the measurement. However, when we perform measurements of momentum for example, we don't assume that the measurement was affected by the device used for it. Indeed we can't continue right afterwards with measurements of position accurately, but still: we consider the value we obtained for the momentum, a quantity that attributed the system at the time of measurement and definitely not device-dependent.

Thus, asserting that time measurements are depended on the apparatus used, we immediately reject that time is a characteristic attribute of the evolving system. Then the time parameter we use inside the Schrödinger equation is just an "external parameter", as it is often described. Something though not particularly convincing if you simply take a look at a list of all these characteristic time observables for various quantum processes, or if you contemplate a bit on how successful the Schrödinger equation have been in describing the evolution of quantum systems.

Moreover, it has to be made clear that the aforementioned scepticism on whether we are able to reach to a probabilistic description of *when* a quantum system can be detected independently or not from the detecting apparatus is not simply a cynic statement, from some strange rejectionists, but from the same people that lead the way of the advancement and the establishment of Quantum Mechanics (Pauli more famously, see (3.1)). And exactly this awe against the "weight of authority" [29, p. 6] is considered by some experts in the field as one of the reasons the further advancement on the problem had been halted for so long.

In conclusion the difficulty insists because it addresses to and challenges both our understanding of time as a concept in Quantum Mechanics and our understating of the very conceptual heart of Quantum Mechanics.

1.1.1 And what's special about the time of arrival?

Probably it is its simplicity, along with its stubbornness for a definite solution, which makes the widely called time-of-arrival problem so widely popular among researchers. It can be defined very accurately, thus it can be tested experimentally accurately too [12, p. 3]. Thus it can be considered as a promising path we can take in pursuing a more conclusive answer to the general problem of time measurements in Quantum Mechanics.

More specifically, we investigate the potentiality of constructing an explicit expression for the probability distribution of the expected time of detection of an emitted ensemble of (quantum) particles or of a single particle moving supposedly towards a specific spatial position, at which point the detector is located. There are many variants of this time-of-arrival problem, from encompassing or not degrees of freedom from detecting apparatus inside the desired probability distribution, to including or not interactions for the particles of the ensemble, between them or from external fields. The simplest case is the free particle case, where no interactions are considered, neither external or between the particles and this is the one considered throughout this whole analysis.

There are two aspects of this specific free particle case that have to be given due weight. One the one hand, that by specifying a spatial position for detection, what we actually require for the particle to be detected is that its quantum state has to be attributed with a specific characteristic, namely its spatial coordinates variables must coincide with these of the spatial point of detection. And on the other hand, the initial conditions of this ensemble of particles have to be determined in order for us to reach to an expression for the probability distribution. By initial conditions again we refer to states attributed with specific values for their parameter values, for example initial momentum value, or initial spatial position value, or even an arbitrary definition of the state with time equals to zero, ie. the beginning of the time measurements. Further remarks on initial conditions of states on Chapter 4.

The rest of the Dissertation focuses specifically on the time-of-arrival problem for the free particle case as a reference to the general topic of time measurements in Quantum Mechanics.

1.1.2 And why do we insist studying it despite the difficulty?

Hopefully we already managed to convey to the reader the significance of studying the time concept in Quantum Mechanics. But what about the significance of the time-of-arrival problem? Is it just the typical persistence of Physicists to give a consistent answer to whichever question are confronted with, even when it comes to a toy model though experiment? Partially this is true, but nowadays reaching to definite answer to the problem will be much assistive for other fields too. As enumerated by Grot et al. [19, p. 2] the reason for studying this problem can be really practical, deeply theoretical or simple because we would like romantically to maintain the prestigious position Quantum Mechanics theory holds in the interpretation of most of the processes of the quantum level. Indeed, it will quite unfair for this theory to manage to have gone thus far, passing through so many theoretical challenges and experimental tests and to fail in the interpretation of such a simplistic process. Quoting Felix T. Smith: "we do not expect that quantum mechanics could fail to predict a probability distribution that can be experimentally measured by simply placing a detector at a fixed position and noting the time at which it "clicks" " [33]. It's just too simple to fail.

Furthermore, apart from the general area of study of time in quantum mechanics, there are adjacent fields which need immediately more specific answers on the perception of time in Quantum Mechanics, in order to contemplate for example on quantum theories in which we don't even consider Newtonian time, quantum gravity be the most significant example [20].

Finally, we can already trace some more practical implications, in contrast to the previous more academic reasons, for example in calculating and simulating rates for chemical reactions. A definite procedure for calculating expressions of probability distributions for the so called *tunnelling time*, the time for which a particle manages to escape through a potential barrier and not its expectation value, ie. the quantity our detectors measure, will allow to even more accurate simulations of chemical reaction processes.

1.2 An overview of the project

This project was assign to the author on the 26th of June 2014 and it was submitted on the 22th of September the same year. It was composed under the supervision of Professor Dr. Jonathan J. Halliwell, who encouraged me choosing a preferable, more specific subject for the project on the general topic of the perception of time in Quantum Mechanics and the time-of-arrival problem. This is not by any means a thorough account on the subject; it's mainly an expression of the level of understanding I managed to reach on the subject, through intensive study of a number of books, thesis and articles, during this very short interval of time.

1.2.1 Goals

This project aims to:

- Introduce even the most unsuspected reader to the difficulties of expressing time measurements in Quantum Mechanics.
- Give to the reader a brief understanding of the necessity for a clearer view on time measurements in Quantum Mechanics.
- Introduce the reader specifically to the additional obstacles one has to confront if we want to express measurements of the time-of-arrival quantity via the standard procedure in Quantum Mechanics, used for so many other measureable quantities.
- Make clear the distinction which is widely used to typically classify the various methods and approaches to the time-of-arrival problem.
- Make clear that the focus is on the so called "ideal" approaches and introduce the reader to a further classification of this category using self-adjointness as a criterion. Of course, as explained later, the latter is not a strict way of distinguish methods, it's mainly schematic for the sake of a more comprehensive presentation.
- Give the reader a clear understanding why a commutation relation for the Hamiltonian operator and an operator of time measurements cannot be primarily considered. This is maybe one of the most important aspects of the whole topic.
- Present briefly historical milestones that played a crucial role for the development of the subject, but which all avoid including self-adjoint expressions of operators inside their analysis.
- Introduce the reader to two highly disputed methods of introducing self-adjoint expressions of operators for an "ideal" perception of time of arrival in Quantum Mechanics. This is the main focus of the whole project and it is presented exhaustively.

- Give finally a brief overview of how delicately one must think when evaluating the conclusions and the results of researches on the area and how much elusive can be to reach to a definite answer for an aspect of the topic.

1.2.2 Structure

There are another four chapters apart from this introductory chapter inside this project. Chapter 2 is the necessary classical reference to the topic of time measurements and the time-of-arrival problem. Chapter 3 presents the "Pauli's Theorem" and significant milestones of the historical development of the topic, giving a view to the reader that in general researches tend to avoid the use of self-adjoint expression for operators in order to reach to probability distributions for the time-of-arrival measurements. Chapter 4 concentrates a great deal of the research effort conducted for this project, even though seemingly the subject of the chapter is very narrowly defined. It presents almost thoroughly the works of two independent teams of researchers on methods of introducing self-adjoint expressions for operators of dimensions of time that eventually, after imposing specific conditions, enable us to construct a specific time-of-arrival probability distribution expression. Chapter 5 is mainly a commentary on Chapter 4 and conclusive remarks.

1.2.3 Prerequisites

Good knowledge of Complex Analysis and Quantum Mechanics are more than sufficient for reading and understanding this project. No exquisite peculiar concepts are needed or introduced. However, a caveat to the reader: the whole topic might seem simple or even simplistic, but it's not. There are very subtle and delicate points inside this analysis, and the reader is encouraged to check for their validity and contemplate carefully upon these by himself.

1.2.4 Acknowledgements

I would like to thank Professor Jonathan J. Halliwell, under the supervision of whom this project was composed and written, firstly for giving me the opportunity to work on this very interesting topic, next for all of his constant encouragement and the freedom he allowed me on choosing a subject on my own and of course for his prompt help on whatever I requested from him.

Also, special thanks to my advisor for the QFFF MSc course, Dr. Timothy Evans, for all the valuable pieces of advice, on dissertation matters as

well, he gave me during the whole past academic year.

1.2.5 Declaration

The following dissertation is my own work; the structure and manner in which concepts are explained is my own, though numerous resources have been used in forming that understanding, and references are given where appropriate. Some sections follow closely the work of others, and are always indicated as such.

Chapter 2

The Classical Reference to the Quantum Problem

"... quantum theory presupposes the classical level... it does not deduce classical concepts as limiting cases of quantum concepts."

— David Bohm (1951) [7]

Despite of the special details of every version of the time-of-arrival problem, all of them refer to the classical description, invoking Bohr's correspondence principle for validity. In this chapter the basic assumptions and relations, and their implications, describing the time-of-arrival problem are presented, giving due weight to the free particle case.

2.1 Formulating the general case

From the definition given to the time-of-arrival problem at the (1.1.1) subsection of the Introduction, we identified the time interval at which the particle is detected, at the position X, with the time-of-arrival quantity (T). For Classical mechanics the time of detection at X coincides with the time the moving particle needs to reach this specific position in space. This is not a valid assumption of course in Quantum Mechanics *a priori* and that's why a clear distinction was made.

The central question in the time-of-arrival problem is if we are capable to predict when a particle is detected, ie. the T quantity, given the initial condition of its movement or of the system it belongs. As mentioned before it's the simplicity of solving this problem classically that makes it so appealing for study and makes us confident that indeed we can reach to a definite answer for it.

Thus, starting with the single-particle case [19], in Classical Mechanics, given specific initial conditions $(q, p) = (q_0, p_0)$, a trajectory for the particle can be definite, uniquely if we refer (if there are any) to conservative interacting fields with the particle. In general thought, a trajectory of the particle $q = q(q_0, p_0, t)$ is the general solution of the equations of motion, with $q = q_0$ and $p = p_0$ for time set to zero, $t = 0$. As a general algorithm again for obtaining the time of arrival for this particle at position $q = X$, which is exactly the same with the time of detection in Classical Mechanics, we can invert (given this is possible) the trajectory equation $q = q(q_0, p_0, t)$ for t in order to obtain an equation of the form: $t = t(q_0, p_0, q)$. Replacing q with the position X of the detector, we have immediately constructed an expression for calculating the classical time-of-arrival quantity:

$$T = t(q_0, p_0, X)\,, \tag{2.1}$$

again provided that the definition of T and $t = t(q_0, p_0)$ coincide.

Multiple crossings

Of course, this inverted equation can be multivalued even with this three arguments q_0, p_0 and X specified exactly. In this case, which is widely called: multiple crossings (for the particle or the ensemble of particles), we are only interested in the lowest value for the time quantity T, ie. the first time the particle crosses X, or as it also widely called the *first-passage time*. For ensembles of n particles, it must be specified if we are interested in the n first-passage times detected, or the first-passage time for each of the n particles. Cases of multiple crossings are definitely out of the scope of this project.

There's another significant attribute of (2.1). Position variables q is defined as real, but it wasn't explicitly specified that its range of values covers the whole axis; maybe it covers a part of it. Thus in case we refer to a position of the detector X out of the range of q, then instead of a real value, we get of course from the inverted equation ((2.1) a complex result. The physical interpretation of this in terms of the time-of-arrival quantity is that for real values of T we refer to positions X that they do can be reached from the particle due to its initial conditions and for complex T values, we refer to position not reachable by the particle. Thus in classical mechanics the distinction between positions and initial conditions that allow detection, from those that do not, is very precise.

2.1.1 Standard Quantization, a brief aside

Observables in Quantum Mechanics are usually associated with self-adjoint operators acting on properly defined quantum states. Its set of eigenvalues from the eigenstates-eigenvalues equation is correspondingly the set of possible values that the observable quantity can exhibit. Also the average expression of the quantum probability distribution of the set of possible observable values is expected to coincide in the classical limit ($\hbar \to 0$) with the value measured or calculated from the classical equations of motion, invoking Borh's correspondence principle and Ehrenfest theorem.

The Standard or Canonical Quantization is a generic heuristic mainly procedure in Quantum Mechanics [27, p. 9] addressing the problem of how to relate classical expressions referring to observable quantities to quantum operators with a proper set of eigenvalues as described before. In plain words, this procedure assumes that a classical expression maintains its validity in the quantum realm translating its canonical variables as operators (quantization). However, it has to be made clear from the start that there's not a single or unique way for doing this. And moreover, different quantizations don't always lead to different result, but they may coincide, as some examples from different quantizations of tunnelling times proved [12].

Hence for the time-of-arrival case the standard quantization would prescribe a substitution of the type:

$$\hat{q}(t) = q(\hat{q}_0, \hat{p}_0, t) \quad \text{and} \quad \hat{T} = t(\hat{q}_0, \hat{p}_0, X)\,, \tag{2.2}$$

where $\hat{q}_0$ and $\hat{p}_0$ are self-adjoint operators of position and momentum correspondingly. However, there's a great difficulty at this point that leads to the aforementioned not-uniqueness on defining operators this way: the ordering of the products of operators when the latter do not commute. Products of operators are not always commutative as this is the case for c-numbers. So which ordering must we choose? This a serious obstacle even for the easiest of the cases, as for example for the free-particle case of the time-of-arrival problem.

2.2 The Free Particle Case

The simplest of the cases, where no interactions at all are assumed. Let particle m which at $t = 0$ is at a position q_0 and it has momentum p_0. Its trajectory equation is simply:

$$q(q_0, p_0, t) = q_0 + p_0 t/m\,. \tag{2.3}$$

Thus, for $q_0 = X$, the inverted equation with reference to t will result to the classical expression for the time of arrival, $T = t(q_0, p_0, X)$:

$$\Rightarrow T = \frac{(X - q_0 m)}{p_0} \tag{2.4}$$

Let's consider, next, an ensemble of non-interacting particles in the free case. We follow for the rest of this subsection the same structure as in Muga and Leavens in [28, p. 360-362]. For classical mechanics, a statistical ensemble of non-interacting particles follows definitely a deterministic motion and by definition Liouville's equation is valid. Let a normalized phase space distribution function $F(q, p, t)$, for which we assume $F(q, p \geq 0, t) = 0$, namely the ensemble moves only to the right of the q axis. Thus we have:

$$\frac{dF(q,p,t)}{dt} = 0 \qquad \text{(Liouville's equation)} \tag{2.5}$$

$$\Rightarrow \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q}\frac{dq}{dt} + \frac{\partial F}{\partial p}\frac{dp}{dt} = 0$$

$$\Rightarrow \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q}\dot{q} + \frac{\partial F}{\partial p}\dot{p} = 0 \tag{2.6}$$

and

$$\int_{-\infty}^{\infty} dq \int_{0}^{\infty} dp F(q,p,t) = 1 \qquad \text{(normalization)} \tag{2.7}$$

2.2.1 The classical time-of-arrival probability distribution

Our aim is to construct an expression of the probability distribution $\Pi(X, T)$ of time of arrival of a particle of the ensemble at a specific spatial position $q = X$. The way we can interpret this probability distribution is that it refers to the probability of detecting a particle (of m mass) of the ensemble (or otherwise the fraction of the ensemble detected) inside the specific spatial range X and $X + dq$ at an arbitrary time interval T and $T + dt$.

Of course the probability for the ensemble to cross a point $X < q_0$ are zero classically since $p_0 > 0$. But we won't assign it though as a condition to the whole setting or we won't confine the time range to positive values mainly for comparison purposes, because the probability for the corresponding quantum-mechanical case is not zero.

Intuitively we can guess what this expression might be, confining firstly the normalization relation (2.7) to the range X and $X+\delta q$ only, per every time interval T and $T+\delta t$:

$$\frac{\int_0^\infty dpF(X,p,T)\delta q}{\delta t}$$

which considerations lead to an expression:

$$\int_0^\infty dp\dot{q}F(X,p,T)\,. \tag{2.8}$$

This product of velocity and probability density resembles to a probability flux expression. But still this is not a strict proof:

Proof of the expression for the current density:. The distribution function $F(q,p,t)$ obeys a continuity equation on the phase space since there aren't any sources or drains:

$$\frac{\partial F(q,p,t)}{\partial t}+\frac{\partial J_q(q,p,t)}{\partial q}+\frac{\partial J_p(q,p,t)}{\partial p}=0\,,$$

where $\vec{J}(q,p,t) = (J_q(q,p,t), J_p(q,p,t))$ is the probability flux or current density of the distribution. Using (2.6) and Hamilton's equations we can compute this current density. Firstly we observe:

$$\begin{aligned}\Rightarrow \frac{\partial F}{\partial t}+\frac{\partial J_q}{\partial q}+\frac{\partial J_p}{\partial p} &= \left(\frac{\partial F}{\partial q}\dot{q}+\frac{\partial F}{\partial p}\dot{p}\right)-\frac{\partial J_q}{\partial q}-\frac{\partial J_p}{\partial p}=0\\ \Rightarrow \left(\frac{\partial(\dot{q}F)}{\partial q}-F\frac{\partial \dot{q}}{\partial q}\right)+\left(\frac{\partial(\dot{p}F)}{\partial p}-F\frac{\partial \dot{p}}{\partial p}\right) &= \frac{\partial J_q}{\partial q}+\frac{\partial J_p}{\partial p}\\ \Rightarrow \frac{\partial(\dot{q}F)}{\partial q}+\frac{\partial(\dot{p}F)}{\partial p}-F\left(\frac{\partial \dot{q}}{\partial q}+\frac{\partial \dot{p}}{\partial p}\right) &= \frac{\partial J_q}{\partial q}+\frac{\partial J_p}{\partial p}\end{aligned} \tag{2.9}$$

and since $\partial/\partial p$ and $\partial/\partial p$ operators commute, we get from Hamilton's equations:

$$\begin{aligned}\frac{\partial H}{\partial q\partial p} &= \frac{\partial H}{\partial p\partial q}\\ \Rightarrow \frac{\partial \dot{q}}{\partial q} &= -\frac{\partial \dot{p}}{\partial p}\Rightarrow \frac{\partial \dot{q}}{\partial q}+\frac{\partial \dot{p}}{\partial p}=0\end{aligned} \tag{2.10}$$

Hence substituting (2.10) to (2.9):

$$\Rightarrow \frac{\partial(\dot{q}F)}{\partial q} + \frac{\partial(\dot{p}F)}{\partial p} = \frac{\partial J_q}{\partial q} + \frac{\partial J_p}{\partial p}$$

and by application of Gauss's theorem:

$$\Rightarrow \int_{-\infty}^{\infty} dq \int_{0}^{\infty} dp \left[\frac{\partial(\dot{q}F - J_q)}{\partial q} + \frac{\partial(\dot{p}F - J_p)}{\partial p}\right] = 0$$
$$\Rightarrow \int_{semi-circle\vec{S}} dq \left[(\dot{q}F - J_q)dS_q + (\dot{p}F - J_p)dS_p\right] = 0 \qquad (2.11)$$

At infinity we don't expect any value for the current, so every contribution comes from the rest, on the $p = 0$ line, thus it is valid to assume: $J_q = \dot{q}F$ and $J_p = \dot{p}F$ □

Therefore we conclude:

$$\Pi(X,T) = \int_{0}^{\infty} dp\, J_q(X,p,T) \equiv J(X,T)\,, \qquad (2.12)$$

where $J(X,T)$ is the current density at spatial point X, for the time interval T to $T + \delta t$. And in order to make a clear connection the initial and general probability density $F(q,p,t)$ and substituting $\dot{q}$ to p/m:

$$\Pi(X,T) = \int_{-\infty}^{\infty} dq \int_{0}^{\infty} dp \frac{p}{m} F(q,p,T)\, \delta(q - X) \qquad (2.13)$$

This is the expression of the classical probability distribution of the time of arrival [27, 28]. It coincides with the intuitive expression (2.8) we constructed and it has the right dimensions of inverse time, namely $\Pi(X,T)\, dT = J(X,T)\, dT$ is the probability detecting a particle (or again the fraction of the ensemble detected) crossing the X to $X + dq$ spatial interval at the T to $T + dt$ time interval.

What if we integrate over all the momentum values?

In case we hadn't assumed in the beginning that $F(q, p \geq 0, t) = 0$, ie. a constraint on the momenta values, we couldn't have taken an expression of the form:

$$J(X,T) = \int_{-\infty}^{\infty} dp\, J_q(X,p,T) = \int_{-\infty}^{\infty} dp\, \frac{p}{m}\, F(X,p,T) \qquad (2.14)$$

as the probability distribution. An example for which its inadequacy is made obvious is the case where we can have the same and opposite contribution to the integral resulting to zero total contribution, ie. particles with same and opposite momenta coming the same time at X. Thus, immediately this renders the above expression as not trustworthy. Of course still, if distinguish between the positive momenta and the negative one, the corresponding current density expressions are perfectly valid:

$$J_+(X,T) = \int_0^\infty dp\, \frac{p}{m}\, F(X,p,T) \tag{2.15}$$

$$J_-(X,T) = \int_{-\infty}^0 dp\, \frac{p}{m}\, F(X,p,T)\,, \tag{2.16}$$

with the drawback though that they are not normalized since they do not refer to the domain in terms of the momenta values. Thus, since the density distribution $F(X,p,T)$ and the mass m are by definition positive, then in order to sum over positive contribution from each term, we can assign a minus sign in front of the second equation, formulating so an acceptable expression for the time-of-arrival probability distribution [28]:

$$\Pi(T,X) = J_+(X,T) - J_-(X,T) = \int_0^\infty dp\, \frac{p}{m}\, F(X,p,T) - \int_{-\infty}^0 dp\, \frac{p}{m}\, F(X,p,T)$$

$$\Rightarrow \Pi(T,X) = \int_{-\infty}^\infty dp\, \frac{|p|}{m}\, F(X,p,T)\,. \tag{2.17}$$

Kijowski's axioms for the classical distribution $\Pi(T)$

For future reference and because of their relevance, it's worthwhile to mention the axioms Kijowski [23] postulated in order to construct immediately through these the probability distribution $\Pi(T)$:

1. The probability distribution is positive throughout its whole domain: $\Pi(T) \geq 0\,,\ \forall\, T \in (-\infty,\infty)$
2. Its time integral equals to the unit: $\int_{-\infty}^\infty dT\, \Pi(X,T) = 1$
3. If we choose another probability density expression such as: $F_1(q + X,p,t) = F(q - X,p,t) =$, then we must have: $\Pi(F_1) = \Pi(F)$, so that X is the fixed position where the measurement takes place.
4. Among any other function that satisfies the above three axioms, we will consider as the probability distribution $\Pi(T)$ the one who results to the minimum value of the expression of the variance of T, $(\Delta(T))^2$.

2.2.2 The classical expression for the average time of arrival

An expression for the classical average time of arrival is important and useful, because many times in Quantum Mechanics we invoke Bohr's correspondence principle, or even Ehrenfest' theorem, in order to justify some of our assumptions and validate results. Also it's the first (order) statistical moment, the existence of which is a good indication that the probability distribution under investigation exists indeed. Hence it is expected that the quantum-mechanical expression for the average time of arrival coincides with the classical one.

We will denote in general (classically or quantum-mechanically) the average time of arrival as $\langle t_A \rangle_X$. By definition the average time-of-arrival expression is obtained by:

$$\langle t_A \rangle_X = \int_{-\infty}^{\infty} dT \, T \, \Pi(X, T) \tag{2.18}$$

In obtaining a simpler expression we have to follow carefully some further steps. For start let's substitute (2.13) inside (2.18), after integrating over the positions:

$$\Rightarrow \langle t_A \rangle_X = \int_{-\infty}^{\infty} dT \, T \int_{0}^{\infty} dp \frac{p}{m} F(X, p, T) \tag{2.19}$$

There's a subtle point here. The way we have to interpret the definition (2.18) is that T now is the random variable, obtaining values through the integration over its whole range; not the resulting value of an expression $T = T(q_0, p_0, 0)$. Hence T has no dependence from momenta values $p = p_0$ and so we can change the order of the two integrations:

$$\Rightarrow \langle t_A \rangle_X = \int_{0}^{\infty} dp \int_{-\infty}^{\infty} dT \frac{Tp}{m} F(X, p, T) \, . \tag{2.20}$$

Then for the equation of motion (2.3): $Tp/m = Tp_0/m = X - q_0$. Again we have to interpret this properly. The time value T multiplied by the momentum of the free particle gave this expression from the equation of motion, in which, since the X value is predefined for the problem, the only variable is the initial position $q_0 = q_0(T, p_0)$, where p_0 can be considered as constant before the integration over momenta values. The differential of q_0, again from the equation of motion, is:

$$\Rightarrow 0 = dq_0 + \frac{p_0}{m} dT \tag{2.21}$$

$$\Rightarrow dq_0 = -\frac{p_0}{m} dT \tag{2.22}$$

Hence, multiplying the differential dT with a factor of $-p_0/m$ we obtain a differential of the initial position q_0.

Again, we have to be careful at this point. The dT differential is positive by definition and the same applies for p_0 and m. Thus we are lead to consider dq_0 differential as negative and so the range of integration is not from $-\infty$ to ∞, but reversed, from ∞ to $-\infty$:

$$\Rightarrow \int_{-\infty}^{\infty} dT \frac{Tp}{m} F(X,p,T) = \int_{-\infty}^{\infty} \left(\frac{dTm}{p_0}\right) \frac{(X-q_0)\,m}{p_0} F(X,p,T)$$
$$= -\int_{\infty}^{-\infty} dq_0 \frac{(X-q_0)\,m}{p_0} F(X,p,T) = \int_{-\infty}^{\infty} dq_0 \frac{(X-q_0)\,m}{p_0} F(X,p,T)$$

Finally we are left to deal with the probability density $F(X,p,T)$. However, invoking again Liouvile's theorem, we are allowed to suppose that the probability density $F(q,p,t)$ at the spatial position X and time T (p arbitrary) is the same for the corresponding initial values of the variables, ie. $F(X,p,T) = F(q_0,p_0,0)$. This 1:1 correspondence of the variables with their initial values of course is an obvious result again of the equation of motion relation (2.3).

Conclusively, (2.19) can be writen as follows, while changing the order of integration since q_0 and p_0 are dependent of each other:

$$\langle t_A \rangle_X = \int_{-\infty}^{\infty} dq_0 \int_0^{\infty} dp_0 \frac{(X-q_0)\,m}{p_0} F(q_0,p_0,0) \tag{2.23}$$

This the final expression of the average time-of-arrival expression [27, 28], which equivalently can be considered as the first statistical moment of the phase-space function $(X-q_0)\,m/p_0$, evaluated with the $F(q_0,p_0,0)$ phase-space density distribution, where we assumed that the singularity at p_0 is cancelled by $F(q_0,p_0,0)$ in order for the integral over momenta to be well defined.

The time integral of the probability distribution $\Pi(T)$

As an aside, it's won't be difficult for the reader to see that by the same method and the normalization condition (2.7), it can be proven that the time integral of the time-of-arrival probability distribution equals to 1:

$$\int_{-\infty}^{\infty} dT\, \Pi(X,T) = \int_{-\infty}^{\infty} dT \int_0^{\infty} dp \frac{p}{m} F(X,p,T) \tag{2.24}$$
$$= \int_{-\infty}^{\infty} dq_0 \int_0^{\infty} dp_0\, F(q_0,p_0,0) = 1\,, \tag{2.25}$$

as expected for a probability distribution of a time quantity.

2.2.3 The difficulty of obtaining a probability distribution in Quantum Mechanics

Following the standard procedure in Quantum Mechanics for constructing a probability distribution of an observable quantity, first a proper self-adjoint operator has to be defined corresponding to the quantity and then its set of eigenstates from the eigenvalue problem have to obtained. Then we construct the probability amplitude for the quantity by projecting the general expression of states defined for the Hilbert space of states onto an eigenstate of the operator. If in the Schrödinger picture, this general state can be considered as the time evolution of an earlier state corresponding to the initial conditions of the problem in consideration. This squared modulus of the complex amplitude is finally the probability distribution for the measurement of the quantity under consideration.

There are in general three main obstacles for reaching to a quantum-mechanical expression for the time-of-arrival probability distribution via the above standard procedure:

- The association of the time-of-arrival quantity with the time parameter of the Schrödinger equation is still highly disputable. Thus assuming the (2.2) identification that $\hat{T} = t(\hat{q}_0, \hat{p}_0, X)$ is not acceptable *a priori*.
- Even if we consider valid to make the above identification, we have to choose an ordering for the constituent operators of the operator expression of the considered time-of-arrival operator. And indeed researchers suggested through time many different expression for such an operator.
- Finally, maybe the severest of the obstacles is the so called "Pauli's Theorem" (3.1), a statement that indicates that the domain of any time operator considered do not coincide with the Hilbert space of state of the problem. Further on this great obstacle in the next chapter.

2.3 The Variety of Approaches

The various methods suggested by researchers in order to deal and give or not an answer to the time-of-arrival problem are usually classified into two categories [29, 32], based on our conceptual incapability described in the introduction of giving a more definite answer on whether or the time-of-arrival measurements are apparatus-independent:

- The "operational approaches", focused on deriving probability distributions which include the behavior of the detection apparatus, even with the simplest detection process.

- The “ideal approaches”, seeking to construct a specific quantum-mechanical operator proper for time-of-arrival measurements and consequently a probability distribution without postulating any degree of freedom from apparatus.

Furthermore, inside this project another classification was applied specifically for the second category of the “ideal approaches”. We distinguished between methods that avoid to use self-adjoint expressions for the “ideal operators” they postulate, and methods that indeed use self-adjoint adjoint operators. The latter is the case by far given prominent weight and studied inside this project.

However, there something that it must be clarified at this point. The distinction between methods that use or not self-adjoint expressions of time-of-arrival operators, is not widely used. Mainly it’s a schematic way of presenting a specific aspect, out of the very wide topic of time in Quantum Mechanics, in order to emphasize that the two works of researchers, exhaustively described inside this project, exhibit this specific attribute that they use self-adjoint expressions for the operators postulated. This is not a strict way of distinguishing the two methods, as there are indeed methods from the two categories far more relevant than others supposedly in the same category, something explicitly shown in the next chapters.

Moreover, the reader mustn’t be misled by the volume dedicated to the chapters 3 and 4 corresponding to each category. This is a project aiming to present extensively methods of self-adjoint operators. However, the truth is that in the general bibliography the methods not using self-adjoint operators supersede in numbers and in the attention given to them the corresponding methods of self-adjoint operators. As an indication we can mention that there are whole reviews on the subject that they only dedicate only a page on the latter methods out of almost a hundred [28]. Hence, it must be clear that this project is dedicated to these few, highly disputable methods.

Chapter 3

Rejecting self-adjointness

"It is surprising that the current mathematical apparatus of quantum mechanics does not include a simple representation for so eminently observable a quantity as the lifetime of metastable entities"

— Felix T. Smith (1960) [33]

Every proper historical review on the topic of time measurements in Quantum Mechanics duly assigns a place as a milestone for the so called "Pauli's Theorem". On hindsight however, many modern researchers agree with this perspective from a rather different point of view. Eric A. Galapon, for example, entitled a 2003 paper of him [16], part of a series of very interesting papers on the subject, as: "What could have we been missing while Pauli's theorem was in force?"; a simple indication of the modern trends on contemplating agian on the "theorem" nowadays.

It's indeed a milestone; nobody has to dismiss this. But from a modern reading it's not only a milestone because of its conceptual and technical contribution to the topic, but rather because of its pessimist undertone which it inherited to whole generations of researchers. And even it might sound peculiar to use sentimental terms as "pessimism" for explaining a certain study direction which a whole topic on Physics had taken, some suggest that it was indeed the heavy name of one the legends of Quantum Mechanics, Wolfgang Pauli himself, that influenced more this evolution of the topic, rather strict scrutiny of every assertion presented, the sacred duty of every scientist. Even this opinion of course, as everything in this topic, is again disputable. In any case, "Pauli's Theorem" was the beginning of a long chain of rejections that time is anything else than an "external parameter" assigned to quantum states and not at all an inherit attribute of these. In other words, let only the clocks to tell the time. Time won't "tell", quoting Prof. J. J. Halliwell.

Then, as the story goes, some "courageous spirits" appeared giving a possible way out to the dead end. They didn't reject the validity of "Pauli's Theorem" itself; they rather rejected the necessity in Quantum Mechanics of associating observables with self-adjoint operators. And it worked. This has been the prominent way of dealing less "pessimistically" with the topic, ie. accepting a certain inherit character of time in quantum evolution.

It's an extensive and truly fascinating subject of the general topic and there's indeed a plethora of this kind of approximations of the problem. In this chapter we are only confined in presenting only two of them, because this projects aims in presenting methods that use self-adjoint expressions of operators. Again, in comparison with the volume of the next chapter, it's not indicative at all of the extent of appreciation these approaches usually receive from the bibliography. The contrary by any standards; methods avoiding self-adjoint expressions is the rule, rather than the exception. Here, only these two methods are presented for the sole purpose of future reference inside this project. And again, distinguishing between methods that use or avoid self-adjoint expressions is mainly a way of presenting the subject in this project, rather than a strict categorization.

3.1 Pauli's "Theorem"

The first thing one has to know about "Pauli's Theorem" is that it is not actually a theorem. And it seems it wasn't intended to be considered as one. It's a footnote on the second article by Pauli inside his famous "Encyclopedia of Physics" (1958) [1]. It's a statement without a strict proof, and as Galapon in the aforementioned series of articles showed [14, 15, 16, 17], there wasn't any rigorous consideration of the domains of the operators. Thus any conclusions Pauli derived from this statement are simply not generally valid. Muga et al., in their historical review, refer to it as a "formal argument" [29, p. 6], while we will refer to this statement as Pauli's "Theorem" from now on, a little bit sarcastically, but not disrespectfully though.

It's historical and conceptual significance again cannot be underestimated because of its proven non-generality and it's always a very good introduction to the technical difficulties and the general problem that lead seemingly unescapably to a dead end. The next is the detailed typical presentation of the statement, where we follow a similar, but more straightforward, structure of a proof as in [12].

3.1.1 Time-energy commutation relation

Let a conservative classical system. We know from Analytical Mechanics that we can describe it using the canonical coordinate variables of position and momentum (q, p). We can also choose another set of coordinate variables to express the behaviour of the system, by imposing a canonical transformation on the initial ones. Choosing specifically energy (through the Hamiltonian) as one of the coordinate variables, we are lead to the time variable as its conjugate. And this due to the following property for the Poisson brackets of the Hamiltonian with another dynamical variable F with no direct time dependence, $F = F(q, p)$ (for a more general treatment, with time dependence for F: [24]):

$$\{H, F(q,p)\} = \frac{dF(q,p)}{dt} ,$$

namely, this specific Poisson brackets is the time derivative of the dynamical variable.

Thus, for an arbitrary variable T conjugate to the Hamiltonian, ie. in terms of the Poisson brackets: $\{H, T\} = 1$, it is straightforward that:

$$\Rightarrow \{H, T\} = 1 = \frac{dT}{dt} .$$

And this arbitrary variable has uniquely dimensions of time and a simple dependence with the time variable of the classical system.

Translating this result to the quantum level, standard (canonical) quantization can be evoked, according to which we replace Poisson brackets to commutators and variables to self-adjoint operators (in the Heisenberg picture)

$$\begin{aligned} \{H, T\} &\rightarrow \frac{1}{i\hbar}[H, T] \\ &\Rightarrow [\hat{H}, \hat{T}] = i\hbar \end{aligned} \tag{3.1}$$

Even though all these considerations seem sufficient for defining a self-adjoint quantum-mechanical operator for time, unfortunately they are not. As Pauli first put forward, assuming self-adjointness for a time operator conjugate to the Hamiltonian operator is in contrast with fact that the Hamiltonian (energy) spectrum is only infinite to the positive values and it is bounded below to the zero value (semi-bounded). And this is definitely not an easily-surpassed obstacle.

An aside on the canonical quantization of the Poisson bracket

It must be stressed that the canonical quantization as described above implies self-adjoint operators for both of the operators for the considered commutator. This is an assumption based mainly on the fact that we postulate a range of values for both the canonical variables on the real axis.

However, assuming or prooving a commutation relation of an operator, say $\hat{A}$, with the Hamiltonian of the form: $[\hat{H}, \hat{A}] = i\hbar$ does not lead to self-adjointness for the $\hat{A}$ operator. This something sometimes misunderstood in the bibliography.

Proof. Let's denote the complex scalar product of two functions of states as: $\langle\phi|\psi\rangle = (\phi, \psi)$ and let's suppose that we have a valid commutation relation: $[\hat{H}, \hat{A}] = i\hbar$, for Hamiltonian $\hat{H}$ and an arbitrary operator $\hat{A}$. The commutator itself of course is not self-adjoint. If it was then by defintion:

$$(\phi, [\hat{H}, \hat{A}]\psi) = \left(\left([\hat{H}, \hat{A}]\right)^{\dagger} \phi, \psi\right) = ([\hat{H}, \hat{A}]\phi, \psi)\,,$$

but since:

$$\left(\left([\hat{H}, \hat{A}]\right)^{\dagger} \phi, \psi\right) = (-i\hbar\phi, \psi) = -i\hbar(\phi, \psi) \qquad \text{and} \tag{3.2}$$

$$([\hat{H}, \hat{A}]\phi, \psi) = (i\hbar\phi, \psi) = i\hbar(\phi, \psi)\,, \tag{3.3}$$

it is obvious that the commutator is not self-adjoint, as expected of course for an imaginary scalar quantity.

But, what about $\hat{A}$ operator? Can we prove its self-adjointness only using the commutation relation? Firstly, let's use the fact that Hamiltonian is indeed self-adjoint. Thus:

$$[\hat{H}, \hat{A}]^{\dagger} = [\hat{A}, \hat{H}] = [\hat{A}^{\dagger}, \hat{H}] \tag{3.4}$$

and replacing then (3.4) inside (3.2) and since (3.2) and (3.3) are actually the same and opposite:

$$\begin{aligned}
\left(\left([\hat{H}, \hat{A}]\right)^{\dagger} \phi, \psi\right) &= ([\hat{A}^{\dagger}, \hat{H}]\phi, \psi) = -i\hbar(\phi, \psi) = -([\hat{H}, \hat{A}]\phi, \psi) \\
&\Rightarrow ([\hat{H}, \hat{A}^{\dagger}]\phi, \psi) = ([\hat{H}, \hat{A}]\phi, \psi) \\
&\Rightarrow ([\hat{H}, (\hat{A}^{\dagger} - \hat{A})]\phi, \psi) = 0
\end{aligned} \tag{3.5}$$

Hence, we reached to equation (3.5), for which we have to investigate if it leads univocally to the self-adjointness of $\hat{A}$. The answer obviously is no.

Operator $\hat{A}$ can be of course self-adjoint, ie. $\hat{A}^\dagger = \hat{A}$ which satisfies equation (3.5), but there are another two possibilities also. Either the difference $\hat{A}^\dagger - \hat{A}$ is a c-number, not an operator, or it's indeed an operator with the same set of eigenvalues, or part of it, with the Hamiltonian operator. Both cases render the commutator with the Hamiltonian as zero.

Therefore, we concluded that the self-adjointness of an arbitrary operator cannot be derived from the commutation relation, but it has to be assumed or proven. □

Finally, from (3.5) we can infer that in general the anti-self-adjoint expression:

$$\frac{\hat{A}^\dagger - \hat{A}}{2} \tag{3.6}$$

commutes with Hamiltonian, while in general again, for every arbitrary $\hat{A}$ operator, the self-adjoint expression:

$$\frac{\hat{A}^\dagger + \hat{A}}{2} \tag{3.7}$$

has exacty the same commutation relation with the Hamiltonian as $\hat{A}$ has. This can be shown if, instead of subtracting, we add equations (3.2) and (3.3), using again (3.4):

$$\Rightarrow ([\hat{H}, (\hat{A}^\dagger + \hat{A})]\phi, \psi) = 2i\hbar(\phi, \psi) \tag{3.8}$$

$$\Rightarrow [\hat{H}, \frac{\hat{A}^\dagger + \hat{A}}{2}] = i\hbar \tag{3.9}$$

3.1.2 Proof of nonexistence according to Pauli

Assuming the existence of a (proper) self-adjoint time operator $\hat{T}$, its eigenstates, $\hat{T}\,|T\rangle = T\,|T\rangle$, will form a complete set of states for the Hilbert space on which they have been defined. The existence of any higher (integer) power for this operator can be also be postulated, by assuming also that it is a well behaved operator. Thus by induction:

$$\hat{T}^n\,|T\rangle = T^n\,|T\rangle \ , n \in \mathbb{N}^0$$

and multiplying each part of the equation with a factor $(i\epsilon/\hbar)^n/n!$, where this ϵ parameter has dimension of energy, then by adding all the possible powers from 0 to ∞ will result to a power series equal to the an exponential function of the time operator:

$$\Rightarrow \sum_{n=0}^{\infty} \frac{(i\epsilon\hat{T}^n/\hbar)^n}{n!} |T\rangle = \sum_{n=0}^{\infty} \frac{(i\epsilon T^n/\hbar)^n}{n!} |T\rangle$$
$$\Leftrightarrow \exp(i\epsilon\hat{T}/\hbar) |T\rangle = \exp(i\epsilon T/\hbar) |T\rangle \tag{3.10}$$

Thus, assuming the validity of the time-energy commutation relation (3.1), a new commutation relation can be inferred, involving this time the exponential operator (3.10). To calculate this commutation relation, we use first a property of the commutators:

$$\Rightarrow [\hat{H}, \hat{T}^n] = i\hbar n\hat{T}^{n-1}\,, \tag{3.11}$$

which leads then for the commutation relation of the Hamiltonian and the exponential operator:

$$\Rightarrow [\hat{H}, \exp(i\epsilon\hat{T}/\hbar)] = [\hat{H}, \sum_{n=0}^{\infty} \frac{(i\epsilon\hat{T}/\hbar)^n}{n!}] = \sum_{n=0}^{\infty} \frac{(i\epsilon T/\hbar)^n}{n!} [\hat{H}, \hat{T}^n]$$
$$= \sum_{n=0}^{\infty} \frac{(i\epsilon/\hbar)^n}{n!} i\hbar n\hat{T}^{n-1} = -\epsilon \sum_{n=0}^{\infty} \frac{(i\epsilon/\hbar)^{n-1}}{n-1!} \hat{T}^{n-1}$$

$$\Rightarrow [\hat{H}, e^{i\epsilon\hat{T}/\hbar}] = -\epsilon\, e^{i\epsilon\hat{T}^n/\hbar} \tag{3.12}$$

So let's consider now the action of this exponential operator on an energy eigenstate $|E\rangle$, using the latter commutation relation (3.12):

$$\Rightarrow e^{i\epsilon\hat{T}/\hbar} |E\rangle = -\frac{1}{\epsilon}[\hat{H}, e^{i\epsilon\hat{T}/\hbar}] |E\rangle = -\frac{1}{\epsilon}(\hat{H}\, e^{i\epsilon\hat{T}/\hbar} - e^{i\epsilon\hat{T}/\hbar}\, \hat{H}) |E\rangle$$
$$= -\frac{1}{\epsilon}\Big(\hat{H}\, e^{i\epsilon\hat{T}/\hbar} |E\rangle - e^{i\epsilon\hat{T}/\hbar}\, E\, |E\rangle\Big)$$
$$\Rightarrow \hat{H}\, e^{i\epsilon\hat{T}/\hbar} |E\rangle = (E-\epsilon)\, e^{i\epsilon\hat{T}/\hbar} |E\rangle \tag{3.13}$$

Therefore, $e^{i\epsilon\hat{T}^n/\hbar} |E\rangle$ expression is an energy eigenstate too, corresponding to the $E-\epsilon$ eigenvalue. And then with the proper normalization we can assert from (3.13) that:

$$\Rightarrow e^{i\epsilon\hat{T}/\hbar} |E\rangle = |E-\epsilon\rangle \tag{3.14}$$

But since there aren't any restrictions for the value of the ϵ parameter, apart from the convergence of the power series, then there aren't any obstacles for these states to be attributed with a negative energy value. Thus, the initial commutation relation (3.1) is not sufficient to restrict the domain of the energy eigenstates to the positive half of the (real) energy axis, but instead, according to (3.14) they have to span, continuously moreover, to the whole axis, ie. $E \in (-\infty, \infty)$. This is contradictory with the by-definition semibound character of the energy spectrum of the states and hence the assumption of the commutation relation (3.1), for this hypothetical self-adjoint time operator, cannot be considered acceptable until this contradiction is settled.

3.2 Two renowned "ideal" suggestions

For future reference, this second part of the chapter refers very very briefly to two quite famous ways of surpassing the difficulties from Pauli's "Theorem" in obtaining probability distributions for the time of arrival as an "ideal" concept, no degrees of freedom from apparatus, without postulating the need for a self-adjoint operator. Again, this is a very extensive topic; the interested reader can consult the bibliography for further study. This is merely a scratch, because this project focuses on another direction on the topic.

3.2.1 Kijowski's axiomatic time-of-arrival probability distribution

On the previous chapter we presented the list of axioms that Kijowski imposed in order to reach successfully and univocally to the classical expression of the time-of-arrival probability distribution. Assuming the same set of axioms for the quantum case, a probability distribution was constructed for a free particle moving in three dimensions [23]. This distribution was originally presented by Allcock [4, 4, 4], through very different considerations, however due to the axiomatic approach, it's more famous because of Kijowski.

Here we skipped the derivation and we are confined to present two versions only of the distribution, for convenience, for one dimensional movement. Hence, for a state $|\psi(t_0)\rangle$ which is a superposition of momentum eigenstates of only positive momenta, it was derived a probability distribution for the arrival time at a spatial position X of the form:

$$\Pi_K[T; X; \psi(t_0)] = \frac{1}{mh} \left| \int_0^{+\infty} dp \sqrt{p} \exp\left(\frac{-iTp^2}{2m\hbar} + ipX \right) \langle p|\psi(t_0)\rangle \right|^2 \quad (3.15)$$

or as function of $k = p/\hbar$ for future reference:

$$\Pi_K[T;X;\psi(t_0)] = \frac{\hbar}{2\pi m}\left|\int_0^{+\infty} dk\sqrt{k}\exp\left(-\frac{i\hbar Tk^2}{2m}+ikX\right)\langle k|\psi(t_0)\rangle\right|^2, \tag{3.16}$$

where t_0 is the initial reference time and it is used notationally instead of $t = 0$ in order for the covariance of the distribution with time translations to be implied explicitly [35], as in the classical case: $\Pi_K[T;X;\psi(t_0)] = \Pi_K[T + t_0;X;\psi(0)]$.

The general relations for states with momenta of any sign is:

$$\Pi_K[T;X;\psi(t_0)] = \frac{\hbar}{2\pi m}\sum_\alpha\left|\int_0^{\alpha\infty} dk\sqrt{\alpha k}\exp\left(-\frac{i\hbar Tk^2}{2m}+ikX\right)\langle k|\psi(t_0)\rangle\right|^2 \tag{3.17}$$

3.2.2 Aharonov-Bohm symmetric time-of-arrival operator

Aharonov and Bohm in their 1961 paper [2] presented a way to measure or calculate time in the quantum level (for various purposes, mainly to argue on the energy-time uncertainty relation) using a free particle as a "clock", simply by measuring its position x and its momentum p_x. This measurement was realized by an operator, which was the symmetrization of the classical expression mx/p_x. Thus correspondingly, for the time-of-arrival quantity, the classical time-of-arrival expression (2.4) was symmetrized and translated properly as an operator expression:

$$\hat{T} = -\frac{m}{2}[(\hat{x} - X)\hat{p}^{-1} + \hat{p}^{-1}(\hat{x} - X)] \tag{3.18}$$

This is not a self-adjoint operator, but a maximally symmetric one, namely almost as useful as a self-adjoint operator.

3.2.3 Giannitrapani and the POVMs

The two methods above were associated together by Giannitrapani in 1997 using the POVM theory [18], by specifically showing that the probability distribution for the Aharonov-Bohm time-of-arrival operator (3.18) coincides with Kijowski's distribution (3.17) [13, 12, 29, 27].

The more interested reader is redirected to the bibliography on the subject.

Chapter 4

Retrieving self-adjointness

"... the introduction of an operator $\hat{T}$ must fundamentally be abandoned..."

— Wolfgang Pauli (1933) [1]

At a later, more recent, point in time, the aforementioned "courageous spirits" of this whole endeavour decided to take another controversial and highly disputable step forward towards the construction of this "ideal" expression for the probability distribution of the time of arrival. They indeed embedded in their considerations and methods properly defined "time" operators with the formerly rejected property of self-adjointness. Of course no self-adjoint time-of-arrival operator, both conjugated and with identical domain of definition to the Hamiltonian, was presented. This is widely still considered non-feasible, or even non consistent with our understanding of Quantum Mechanics. What the researchers suggested inside their works was the construction of expressions of self-adjoint operators with dimensions of time that are used carefully to the end of the construction of the desired probability distribution.

More specifically, in this chapter we present the works of two independent teams of researchers, N. Grot, C. Rovelli and R. S. Tate [19] (and partially [31]) in the first section, and V. Delgado and J. G Muga [12] in the second. The main idea that allows us the association of these two papers including them as a whole in a chapter is based on two facts. That, on the one hand, the reason that Pauli's "theorem" (3.1) prohibits a $[\hat{H}, \hat{T}] = i\hbar$ commutation relation is due to the semi-bounded character of the Hamiltonian energy spectrum and that, on the other hand, it was proven recently [14, 15, 16, 17], that the consideration of bounded (this time) self-adjoint time-of-arrival operators, conjugated to the Hamiltonian, is indeed consistent with its semi-bounded energy spectrum.

Taking these into account, it can become evident that the introduction of a self-adjoint operator of dimensions of time conjugated to the Hamiltonian can be achieved through two paths. Either we can change the range of definition on the Hilbert space of states for the time-of-arrival operator we postulated, modifying the operator this way, turning it into a new bounded "time" operator, while leaving the Hamiltonian as it is. Or we can expand the defining set of states for the Hamiltonian operator this time, in order to incorporate states (of negative energy) prohibited before, modifying this way both the Hamiltonian to a new energy operator and also the time-of-arrival operator to a new self-adjoint "time" operator.

The resulting new operators corresponding to the time-of-arrival concept are self-adjoint, thus they do can straightforwardly lead to a probability distribution, more easily of course for the simple case of a free quantum particle. Applying then proper conditions in each case, we can associate these final distributions of the modified operators with the desired time-of-arrival probability distribution. The results of the two different methods in terms of the final time-of-arrival probability distribution amazingly coincide and they are identical to the Kijowski's distribution. Further remarks on the two methods continue on Chapter 5, where also it is made apparent why these results coincide.

Again it has to be said, as explained in the Introduction, that in this project the whole classification into methods that use or avoid self-adjoint "time operators" is in the most degree schematic, mainly for the sake of a proper presentation, aligned with the goals of the whole project. The two works considered relevant in this chapter, they might have been considered diverging in another context, in a classification of different criteria.

4.1 Modifying the time-of-arrival operator

Grot et al. in their 1996 paper [19] manage to reach to an expression for the time-of-arrival probability distribution for the free particle case (no degrees of freedom from apparatus were postulated), through the construction of a self-adjoint operator of dimensions of time, which is the proper modification of the postulated expression for the time-of-arrival operator. The confined domain of the initial time-of-arrival operator is expanded for the definition of the new "time" operator, in an attempt to coincide with the domain of the Hamiltonian operator. The Hamiltonian remains unmodified throughout the whole analysis.

4.1.1 Basic definitions and relations

Firstly, let's assume that indeed a self-adjoint time-of-arrival operator $\hat{T}$ exists in general (for the free case or not), as an "ideal" concept, namely that it corresponds to measurements of the time-of-arrival quantity independent of the measuring apparatus used. The eigenvalue equation of the operator $\hat{T}|T\rangle = T|T\rangle$ produces its set of eigenstates $\{|T\rangle\}$.

The projection of a state from the Hilbert space of states onto an eigenstate $|T\rangle$ results to the probability amplitude $\psi(T)$. The probability distribution $\pi(T)$ is of course the squared modulus of this complex amplitude:

$$\pi(T) = |\psi(T)|^2 = \overline{\psi(T)}\psi(T)$$
$$\Rightarrow \pi(T) = \overline{\langle T|\psi\rangle}\langle T|\psi\rangle = \langle\psi|T\rangle\langle T|\psi\rangle = \langle\psi|\Big(|T\rangle\langle T|\Big)|\psi\rangle \tag{4.1}$$

Definiing then the projector operator:

$$\hat{P}(T) \equiv |T\rangle\,\langle T|\ , \tag{4.2}$$

the expression for the probability distribution (4.1) then becomes:

$$\Rightarrow \pi(T) = \langle\psi|\hat{P}(T)|\psi\rangle \tag{4.3}$$

A self-adjoint operator as an expansion of its eigenstates

The eigenstates of a generally well-defined self-adjoint operator $\hat{A}$ form a complete set of states. Integrating thus its projector operator gives the identity operator:

$$\int_{-\infty}^{\infty} dA\,|A\rangle\,\langle A| \equiv \int_{-\infty}^{\infty} dA\hat{P}(A) = \hat{1}\,. \tag{4.4}$$

Using (4.4) an expression for the self-adjoint operator can be obtained, using the definition of the average value of a measurable quantity:

$$\langle A\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}\,\hat{1}|\psi\rangle = \langle\psi|\hat{A}\int_{-\infty}^{\infty} dA\,|A\rangle\,\langle A|\,\psi\rangle$$
$$= \langle\psi|\int_{-\infty}^{\infty} dA\,\hat{A}\,|A\rangle\,\langle A|\,\psi\rangle = \langle\psi|\int_{-\infty}^{\infty} dA\,A\,|A\rangle\,\langle A|\,\psi\rangle \tag{4.5}$$

Therefore we get:

$$\hat{A} = \int_{-\infty}^{\infty} dA\,A\,|A\rangle\,\langle A| = \int_{-\infty}^{\infty} dA\,A\hat{P}(A) \tag{4.6}$$

4.1.2 Redefining the domain of the $\hat{T}$ operator

It's obvious that relation (4.6) is valid only for the cases of a complete set of eigenstates. And Grot et al. warn us to avoid the temptation of defining analogously the time-of-arrival operator, even if it admits real eigenvalues, even if it is seemingly self-adjoint, ie. $\hat{T} = \hat{T}^{\dagger}$, because the "spectral family", as they call the $\hat{P}(T)$ operator (4.2) is not complete on the whole Hilbert space of states. The only restrictions for the $\{|\psi\rangle\}$ states of the Hilbert space are maybe some initial conditions or any considered interactions with the particle, while there are more restrictions on the $\{|T\rangle\}$ states.

Hence the domain for which the time-of-arrival operator $\hat{T}$ is defined is a subset of the whole Hilbert space of states for the particle, for which the Hamiltonian $\hat{H}$ is defined, because there are states for which the particle cannot be detected at the predefined spatial position X (in correspondence with the classic case). Thus the Hillbert space $\mathcal{H}$ can be split into a $\mathcal{H}_{detected}$ part and a $\mathcal{H}_{never\,detected}$ part. In other words $\mathcal{H}_{detected}$ constitutes of states with positive time of detection and $\mathcal{H}_{never\,detected}$ of states with zero and negative time of detection, the latter *a priori* postulated unphysical.

Remarks on the two components of the Hilbert space and on the initial conditions

Another subtle point of the Grot et al. analysis is that they consider these two sections of the Hilbert space of physical states of the particle as orthogonal to each other, on the basis of the validity of the superposition principle for the probability distribution. The validity of the principle is left to be decided under the experimental scrutiny; however the authors consider it reasonable to be postulated. In other words, whether there are states never detectable indeed (ie. not small, zero possibility), has to be left to the experimentalists.

Of course this strict separation between the states of the Hilbert space characterized by a specific measurable attribute, the time of detection of the particle, immediately leads to the question on the accuracy of this definition. How can we be sure that we can't get "detection-before-preparation" states, as the authors put it? Assuming, for example, $|x_0; p_0\rangle$ as the initial state for a particle, for x_0 and p_0 that classically allow the particle to reach X, this state might be a superposition of $|T\rangle$ eigenstates or it might not be possible to be expanded in $|T\rangle$ eigenstates because it consists partially of a superposition of some states of the $\mathcal{H}_{never\,detected}$.

How do we define then carefully the initial conditions? The authors answer this question in correspondence with the classical case. In the classical case we set that the beginning of the time measurements, at $t = 0$, is for initial conditions x_0 and p_0, which will define the motion of the particle uniquely, with the assumption though that these initial conditions not being disturbed at all. Quite the same for the quantum analogue. If T the time of arrival for a particle, then we can assume that at a much earlier time in the past t, the particle was in such a state $\psi(t)$ (Schrödinger picture), evolved uniquely to the $\psi(t = 0)$ state, because it wasn't disturbed at all. In other words, we won't measure initial conditions, we will set them long before and arrange for the particle not to be disturbed while reaching these initial conditions.

An expression for the average time-of-arrival

Returning back to the projector operator, it's now clear that integrating the spectral projectors from $-\infty$ to ∞ won't give the unity operator as in (4.4), because, as mentioned before, the eigenstates of the $\hat{T}$ operator do not form a complete set for the whole Hilbert space.

$$\hat{P} \equiv \int_{-\infty}^{\infty} dT \, |T\rangle \, \langle T| \equiv \int_{-\infty}^{\infty} dT \hat{P}(T) \neq \hat{1} \, . \tag{4.7}$$

Instead the action of this $\hat{P}$ operator on the states $|\psi\rangle$ of the particle will project onto states belonging to the $\mathcal{H}_{detected}$ section, while the action of its complement $\hat{1} - \hat{P}$ will project to the $\mathcal{H}_{never\,detected}$ states.

Thus again, an expression for the operator as an expansion of its eigenstates cannot be obtained using (4.6), ie. the expression:

$$\int_{-\infty}^{\infty} dT \, \hat{T} P(T)$$

is by no means an expression for the time-of-arrival operator.

Despite these, we are able thought to construct an expression for the very useful quantity of the average of the time of arrival:

$$\langle \hat{T} \rangle_\psi = \frac{\langle \psi | \hat{P} \, \hat{T} \, \hat{P} | \psi \rangle}{\langle \psi | \hat{P} | \hat{P} | \psi \rangle} = \frac{\langle \psi | \hat{P} \, \hat{T} \, \hat{P} | \psi \rangle}{\langle \psi | \hat{P} | \psi \rangle} \, , \tag{4.8}$$

since, of course, $\hat{P}^2 = \hat{P}$.

On the self-adjointness of the $\hat{T}$ operator with confined domain

It has to be made clear that, even if we have confined the domain of definition of the $\hat{T}$ operator to the $\mathcal{H}_{detected}$ part of the Hilbert space of states, we still cannot consider the operator as self-adjoint. It can be misleading the fact that these $\mathcal{H}_{detected}$ states correspond to real (ie. measureable) values for the time-of-arrival quantity or that we do can find a basis for expressing these states such that the eigenstates of the $\hat{T}$ operator are diagonal or even that the action of the (4.7) operator on the $\mathcal{H}_{detected}$ state projects again on the $\mathcal{H}_{detected}$ space. Still, they do not suffice for characterizing $\hat{T}$ as self-adjoint, since the actual and accurate definition of self-adjointness for $\hat{T}$ would have been:

$$\left(\langle\psi|\hat{T}^{\dagger}\right)|\psi\rangle = \langle\psi|\left(\hat{T}|\psi\rangle\right), \tag{4.9}$$

with the $\{|\psi\rangle\}$ states defined on the whole Hilbert space, not only on $\mathcal{H}_{detected}$. Thus, since the domains of definition do not coincide, the relation fails to be valid.

4.1.3 The $\hat{T}$ operator for the free particle case

Again we consider the free particle case, as defined in detail in the Chapter 2, $\hat{H} = \hat{p}^2/2m$ the free Hamiltonian and the classical expression for the time of arrival at a certain spatial position X:

$$T(X) = \frac{m(X - x_0)}{p_0} \tag{4.10}$$

Obviously, expect from the case for $p_0 = 0$ the particle is expected to reach point X and thus be detected for any other initial conditions for x_0 and p_0, something that allows to postulate that the range of the Hilbert space of states for the free particle (except again for the $p_0 = 0$ case) coincides almost with the domain of the $\hat{T}$ operator. This is very useful, since we don't have to investigate more for any finite regions of momentum for which the corresponding momentum states are considered non-physical.

We reach again the point where we have to decide the way we have to translate the classical expression to a quantum-mechanical expression of operators (in the Heisenberg picture). Of course again the problem is the fact that the quantum-mechanical operators (and their functions of operators) corresponding to the variables of the classical expression (4.10) do not commute with each other. And in the specific case the operators for the initial spatial position x_0 and the initial momentum p_0 (and any functions of these) do not commute of course:

$$\begin{aligned} [\hat{x}_0, \hat{p}_0] &= i\hbar \\ \Rightarrow [\hat{x}_0, f(\hat{p}_0)] &\neq 0 \\ \Rightarrow \left[\hat{x}_0, \hat{p}_0^{-1}\right] &\neq 0 \end{aligned}$$

Hence, in invoking the correspondence principle we have to also choose an ordering for the operators, since for the operators involved we've proven that their ordering matters, and as explained before, this choice of ordering is far from unique. Thus, Grot et al. made a specific choice of ordering for the expression $\hat{T}(\hat{x}_0, \hat{p}_0)$, on the grounds of convenience for calculations, on the one hand, and on consistency, on the other hand, with the desired self-adjoint character for the operator.

Explaining the latter, let's remember firstly that x_0 and p_0 are themselves self-adjoint operators, but any simple product of any ordering of them is not. Hence, we need an expression of these operators in an ordering which must be in overall self-adjoint and of course that will coincide with the classical expression in the classical limit. And since the adjoint of an operator expression has the ordering of its constituent operators reversed, thinking simply, we would say that a symmetric expression for these constituent operators, quite similarly to the Aharonov-Bohm symmetric operator (3.18), would be very promising for constructing a self-adjoint operator.

We can observe next that an expression which splits one of the constituent operators into square roots can be symmetric indeed: $\sqrt{x_0}\,(p_0)^{-1}\sqrt{x_0}$ or $(\sqrt{p_0})^{-1} x_0 (\sqrt{p_0})^{-1}$. These are both obviously symmetric if we reverse their order (again up to $p_0 = 0$). However, Grot et al. chose the latter expression from the two, mainly for reasons of convenience in calculations. This is made straightforwardly obvious when considering expressing the x_0 and p_0 operators in the momentum basis which basis diagonalizes p_0 (again in the Heisenberg picture):

$$\hat{x}_0 \psi(k) = i \frac{d}{dk} \psi(k) \tag{4.11}$$

$$\hat{p}_0 \psi(k) = \hbar k \psi(k) \tag{4.12}$$

The square root of the momentum operator can be more easily treated, than the square root of position, in the momentum basis.

Hence, with all these considerations Grot et al. manage to construct a convenient self-adjoint expression for the $\hat{T}$ operator from the classical expression (4.10) in the momentum basis using (4.11) and (4.12):

$$\Rightarrow \hat{T}(X)\psi(k) = \left[\frac{mX}{\hbar k} - i \frac{m}{\hbar} \frac{1}{\sqrt{k}} \frac{d}{dk} \frac{1}{\sqrt{k}} \right] \psi(k)\,, \tag{4.13}$$

defined on the whole momentum spectrum, apart from the $k = 0$ value. The square root for negative values of k was taken as: $\sqrt{k} = i\sqrt{|k|}$.

Furthermore, using the unitary operator for spatial translations, $e^{-i\hat{P}X}$:

$$\hat{T}(X) = e^{-i\hat{P}X} \hat{T}(0)\, e^{i\hat{P}X} \tag{4.14}$$

we can obtain a corresponding operator $\hat{T}(0)$ for measurements (detection) on the origin. Therefore, without any loss of generality, we can work with the operator $\hat{T} \equiv \hat{T}(0)$ which has the simpler form (again in the momentum basis):

$$\Rightarrow \hat{T} = -i\frac{m}{\hbar}\frac{1}{\sqrt{k}}\frac{d}{dk}\frac{1}{\sqrt{k}}\,, \quad (k \neq 0)\,. \tag{4.15}$$

An expression then for the eigenfunctions of the (4.15) operator in the momentum representation (again excluding the $k = 0$ case) is easily calculable [19, p. 7]:

$$g_T(k) = A_{\pm}\sqrt{\frac{\hbar}{2\pi m}}\sqrt{k}\exp\left(\frac{i\hbar T k^2}{2m}\right)\,, \tag{4.16}$$

where $A_{\pm}$ are constant normalization factors only dependent of the sign of the momentum value k, not on the value k itself. This distinction exists because the operator $\hat{T}$ changes sign for $k < 0$ and as Oppenheim et al. [31] note, $\hat{T}$ not only changes sign, but it does it discontinually.

It shouldn't come as a surprise to the reader that these eigenfunctions are not orthogonal, since $\hat{T}$ is not self-adjoint (see 4.1.2). However, the latter casts away any hopes that the $\hat{T}$ operator as expressed in the momentum representation might be self-adjoint. In conclusion, $g_T(k)$ eigenstates are not suitable for constructing the probability distribution of the time of arrival via the standard procedure of Quantum Mechanics.

An aside on the reasons for the non-orthogonality of the $g_T(k)$ states

At this exact point it's worthwhile to mention another disagreement between Grot et al.'s and Oppenheim et al.'s [31, p. 3,4] analysis, on the reasons why the $g_T(k)$ eigenfunctions are not orthogonal. Grot et al. assume without proof that again the singularity $k = 0$ prevents the $g_T(k)$ states from being orthogonal. Oppenheim et al. instead reject this explanation as partial and go even further stating with a simple proof that the reason actually is the fact that the $\hat{T}$ operator (of the free particle case) and its adjoint $\hat{T}^{\dagger}$ are defined in different domains on the Hilbert space of states.

Proof. Let square integrable and differentiable arbitrary functions $u(k)$ and $v(k)$. Denoting the complex scalar product as:

$$\langle u|v\rangle = \int dk\overline{u(k)}v(k)\,,$$

we investigate the result of the following difference, which of course is expected to be zero, it's simply the definition of the adjoint of an operator:

$$\langle u|\hat{T}v\rangle - \langle \hat{T}^{\dagger}u|v\rangle =$$
$$\int dk \left[\overline{u(k)}\Big[-i\frac{m}{\hbar}\frac{1}{\sqrt{k}}\frac{d}{dk}\Big(\frac{1}{\sqrt{k}}v(k)\Big)\Big] - \overline{\Big[-i\frac{m}{\hbar}\frac{1}{\sqrt{k}}\frac{d}{dk}\Big(\frac{1}{\sqrt{k}}u(k)\Big)\Big]}v(k)\right]$$
$$= -i\frac{m}{\hbar}\int dk \left[\frac{\overline{u(k)}}{\sqrt{k}}\frac{d}{dk}\left(\frac{v(k)}{\sqrt{k}}\right) + \frac{d}{dk}\left(\frac{\overline{u(k)}}{\sqrt{k}}\right)\frac{v(k)}{\sqrt{k}}\right]$$
$$= -i\frac{m}{\hbar}\int dk \left[\frac{d}{dk}\left(\frac{\overline{u(k)}v(k)}{k}\right)\right].$$

In order to deal with the singularity for $k = 0$, we split the integral:

$$= -i\frac{m}{\hbar}\left[\int_{-\infty}^{0^-} dk\,\frac{d}{dk}\left(\frac{\overline{u(k)}v(k)}{k}\right) + \int_{0^+}^{\infty} dk\,\frac{d}{dk}\left(\frac{\overline{u(k)}v(k)}{k}\right)\right].$$

And assuming a good asymptotic behaviour for the $u(k)$ and $v(k)$ at infinity:

$$= -i\frac{m}{\hbar}\left(\left[\frac{\overline{u(k)}v(k)}{k}\right]_{-\infty}^{0^-} + \left[\frac{\overline{u(k)}v(k)}{k}\right]_{0^+}^{\infty}\right)$$
$$= -i\frac{m}{\hbar}\left(\lim_{k\to 0^-}\frac{\overline{u(k)}v(k)}{k} - \lim_{k\to 0^+}\frac{\overline{u(k)}v(k)}{k}\right)$$
$$= i\frac{m}{\hbar}\left(\lim_{k\to 0^+}\frac{\overline{u(k)}v(k)}{k} - \lim_{k\to 0^-}\frac{\overline{u(k)}v(k)}{k}\right)$$
$$\Rightarrow \langle u|\hat{T}v\rangle - \langle \hat{T}^{\dagger}u|v\rangle = i\frac{m}{\hbar}\left(\lim_{k\to 0^+}\frac{\overline{u(k)}v(k)}{|k|} + \lim_{k\to 0^-}\frac{\overline{u(k)}v(k)}{|k|}\right) \tag{4.17}$$

Hence, in investigating what prevents this difference from being equal to zero, we observe that the factor $1/|k|$ is not the only "problematic" term in the expression. Indeed, this factor forces us to exclude from the defining domain of $\hat{T}$ any state function for which the expression (4.17) diverges to infinity at $k = 0$, but there's another subtle "problematic" point.

Even if we confine $\hat{T}$ to be defined in a set of states "well behaved" in terms of the $1/|k|$ factor, in order for (4.17) to be zero the expression $\overline{u(k)}v(k)/|k|$ must be additionally continuous at $k = 0$ and odd. And this a fact that clearly sets some further conditions on the allowed state functions for the domain of the $\hat{T}$ operator. However, the requirement for $\overline{u(k)}v(k)$ to be specifically odd, leads to the next requirement that if one of the functions is odd, then the other is necessarily even and vice versa. Thus there's another condition on the allowed functions, even more confusing, because it sets different restrictions on the domain of the $\hat{T}$ operator and different restrictions for the domain of the $\hat{T}^\dagger$ operator.

In conclusion, defining $\hat{T}$ on the whole Hilbert space, while excluding diverging states for the singularity case $k = 0$ does not in any way lead to self-adjointness for the operator and thus the $k = 0$ singularity is not the only root of the evil.

□

4.1.4 The time-of-arrival probability distribution

It should be obvious by now that what prohibits us from the straightforward application of the relation (4.3), for the construction of the probability distribution expression for the free case, is that still even in the free case the operators $\hat{H}$ and $\hat{T}$ have different domains of definition. The $k = 0$ singularity forces the exclusion of some states of $\mathcal{H}$ from the domain of the $\hat{T}$ operator and thus (4.3) is simply not valid. Temptations like, confining $\{|\psi\rangle\}$ states too on the $\mathcal{H}_{detected}$, are only theoretical games, not actually feasible; for example how can we exclude this and only the $k = 0$ component from a Gaussian wave packet?

The regulated modification of $\hat{T}$ and its eigenfunctions

Hence, the ideal situation for the construction of the desired distribution would have been if we had an operator corresponding to the time-of-arrival quantity under investigation, defined in the same domain as the Hamiltonian $\hat{H}$ and which it would have been of course self-adjoint. Seemingly the only obstacle is this $k = 0$ singularity. Thus, Grot et al. [19, p. 7] suggested a way out of this dead end, by a reasonable expansion of the definition of the $\hat{T}$ operator in an attempt to circumvent the $k = 0$ singularity case and which succeeds in being self-adjoint.

The main idea was to construct a modified expression for the $\hat{T}$ operator, similar to the one already obtained, and which in the classical limit approximates arbitrarily closely the classical expression for the time-of-arrival (ie. the average value expression of the modified operator still equals the value of the classical time of arrival). The suggested modified operator $\hat{T}_\epsilon$ by the authors is:

$$\hat{T}_\epsilon = -i\frac{m}{\hbar}\sqrt{f_\epsilon(k)}\frac{d}{dk}\sqrt{f_\epsilon(k)}\,, \tag{4.18}$$

where:

$$f_\epsilon(k) = \begin{cases} \frac{1}{k}\,, & \text{for } |k| > \epsilon \\ \epsilon^{-2}k\,, & \text{for } |k| < \epsilon \end{cases} .$$

and ϵ an arbitrary small parameter. Thus $\hat{T}$ and $\hat{T}_\epsilon$ remain identical for values of momenta away from the $k = 0$ value and for low momenta values, the k^{-1} factor is replaced by a $\epsilon^{-2}k$ expression.

This procedure in general is called "regulation" and it is out of the scope of this presentation to refer any further. What is really important to be mentioned though is that the authors managed to construct for this regulated operator a set of eigenstates in the momentum basis. Their explicit expression for the $|k| > \epsilon$ region of the momentum spectrum is:

$$g^{\pm}_{T_\epsilon}(k) \equiv \langle k|T;\pm\rangle_\epsilon = A_\pm\sqrt{\frac{\hbar}{2\pi m}}\sqrt{k}\exp\left[\frac{i\hbar T(k^2-\epsilon^2)}{2m}\right], \tag{4.19}$$

where $\{|T;\pm\rangle_\epsilon\}$ are the eigenstates of the $\hat{T}_\epsilon$ operator. By the above definition of the operator (4.18), the $\{|T;\pm\rangle_\epsilon\}$ states are defined continuously on the momentum spectrum.

This $\pm$ sign refers again to the sign of momenta values and its necessity is made obvious when we observe the 2:1 degeneracy of the eigenvalues of $\hat{T}_\epsilon$ on the momentum spectrum (ie. the $\pm k$ momenta correspond to the same T value). So we would like to explicitly refer to which sign of momenta we are dealing with each time and that's why the $\pm$ notations. A simple way to observe this degeneracy of the $\hat{T}_\epsilon$ eigenvalues is by noticing that the $\hat{T}_\epsilon$ operator simply changes sign for negative momenta. The expression remains the same with a different sign for the corresponding $\pm k$ values. Thus the eigenvalue is the same for $\pm k$.

If more strictly we want to prove that a $|T;\pm\rangle_\epsilon$ state consists of momenta states of only a specific sign (eg. positive), we can start by noticing that the $\hat{T}_\epsilon$ operator (through its whole k spectrum) and the sign operator $\Theta(k) = \text{sgn}(k) = k/|k|$ commute. Thus an eigenfunction of $\hat{T}_\epsilon$ is simultaneously an eigenfunction of the sign operator and this implies that a $\hat{T}_\epsilon$ eigenfunction can be expanded in terms of eigenfunctions of the $\hat{k} \equiv \hat{P}/\hbar$ operator, with support on the k momentum spectrum only on the positive or only on the negative values.

There are next two aspects of the (4.19) result for the eigenstates of the $\hat{T}_\epsilon$ operator which justify its significance. First of all, it's the fact that their dependence on this ϵ parameter can be factored out, because it's inside the exponential term, and hence its actual contribution to the initial $g_T^{\pm}(k)$ eigenstates (4.16) is simply up to a phase term:

$$\Rightarrow g_{T_\epsilon}^{\pm}(k) = A_{\pm}\sqrt{\frac{\hbar}{2\pi m}}\sqrt{k}\exp\left(\frac{i\hbar T k^2}{2m}\right)\exp\left(\frac{-i\hbar T \epsilon^2}{2m}\right), \tag{4.20}$$

This is exactly what will make the rest of the calculations very easy to handle.

Secondly, it's the fact that these $g_{T_\epsilon}^{\pm}(k)$ eigenstates are orthogonal for the whole momentum spectrum, justifying this way the specific choice of regulation the authors made. There's a detailed proof of this magnificent attribute of these states [19, p. 9,10] and indeed this fact is a clear indication that the $\hat{T}_\epsilon$ is self-adjoint (since it's defined for the whole Hilbert space of states) and its eigenstates then can be used for the construction of an explicit expression of the operator as in (4.6), alongside with the calculation of other quantities such as the probability amplitude. And remembering that $\hat{T}$ and $\hat{T}_\epsilon$ are identical for large enough momenta, constructing the desired probability distribution for this region of the momenta spectrum is straightforward now.

The final expression of the probability distribution

As described above, following the standard procedure in quantum mechanics (in the Heisenberg picture), the probability amplitude is obtained by the projection of the states of the Hilber space onto the eigenstates of the operator. Hence for the $\{|T;\pm\rangle_\epsilon\}$ states we refer to an expression of the form: ${}_\epsilon\langle T;\pm|\psi\rangle$, which expression we can split: ${}_\epsilon\langle T;\pm|\psi\rangle = {}_\epsilon\langle T;+|\psi\rangle + {}_\epsilon\langle T;-|\psi\rangle$ (due to the orthogonality of the $\{|T;\pm\rangle_\epsilon\}$ states). Using the completeness relation for the momentum eigenstates, we can calculate this amplitude using the (general) $g_{T_\epsilon}^{\pm}(k)$ states:

$${}_\epsilon\langle T;\pm|\psi\rangle = {}_\epsilon\langle T;\pm|\int_{-\infty}^{\infty} dk\,|k\rangle\,\langle k|\,|\psi\rangle = \int_{-\infty}^{\infty} dk g_{T_\epsilon}^{\pm}(k)\psi(k) \tag{4.21}$$

And since the probability distribution is the squared value of the (complex) amplitude, $\pi(T) = |{}_\epsilon\langle T;\pm|\psi\rangle|^2$, then:

$$\Rightarrow \pi(T) = \left|\int_{-\infty}^{\infty} dk g_{T_\epsilon}^{\pm}(k)\psi(k)\right|^2$$

$$\Rightarrow \pi(T) = \left|\int_{0}^{\infty} dk g_{T_\epsilon}^{+}(k)\psi(k)\right|^2 + \left|\int_{-\infty}^{0} dk g_{T_\epsilon}^{-}(k)\psi(k)\right|^2 \tag{4.22}$$

due to the proven orthogonality of the $g_{T_\epsilon}^{\pm}(k)$ states again.

Hence substituting (4.20) to (4.22), the phase term containing the ϵ parameter (and not any expression of k) vanishes immediately. We get then a much more simple expression, without any ϵ dependence, for which, if we consider ϵ very small, we are allowed to take 0 as one of the limits of the integration. Still, of course, the final expression won't be valid for the case of a zero-velocity particle (ie. on the detector):

$$\Rightarrow \pi(T) =$$
$$\frac{\hbar}{2\pi m}\left(\left|\int_0^{\infty} dk\sqrt{k}\exp\left(\frac{i\hbar T k^2}{2m}\right)\psi(k)\right|^2 + \left|\int_{-\infty}^{0} dk\sqrt{k}\exp\left(\frac{i\hbar T k^2}{2m}\psi(k)\right)\right|^2\right),$$

Or more concisely, if we distinguish between the cases of well-defined positive momentum direction to the corresponding negative ones:

$$\Rightarrow \pi^{\pm}(T) = \frac{\hbar}{2\pi m}\left|\int_0^{\pm\infty} dk\sqrt{k}\exp\left(\frac{i\hbar T k^2}{2m}\right)\psi(k)\right|^2 . \tag{4.23}$$

This is of course the case where the detector is located on the origin. For detection in another spatial position X we have to apply a spatial translation transformation to the eigenstates of the T_ϵ operator

$$|T;\pm;X\rangle_\epsilon \equiv e^{-i\hat{P}X/\hbar}\,|T;\pm\rangle_\epsilon , \tag{4.24}$$

which in the momentum basis:

$$\Rightarrow g^{\pm}_{T_\epsilon;X}(k) = \langle k|T;\pm;X\rangle_\epsilon = e^{-ikX} g^{\pm}_{T_\epsilon}(k) . \tag{4.25}$$

Thus, using (4.25) as the expression for the eigenstates of the $\hat{T}_\epsilon$ operator in the momentum basis, we reach to the final expression, according to Grot et al., for the probability distribution of the time of arrival T of a free quantum particle with well-defined momentum direction, positive or negative, at a specific spatial position X:

$$\boxed{\Rightarrow \pi^{\pm}(T) = \frac{\hbar}{2\pi m}\left|\int_0^{\pm\infty} dk\sqrt{k}\exp\left(\frac{i\hbar T k^2}{2m} - ikX\right)\psi(k)\right|^2} \tag{4.26}$$

which is obviously identical to Kijowski's distribution (3.16).

Computational application with a Gaussian wave packet

As a very interesting application of the result of their analysis, Grot et al. calculated computationally the probability distribution of the time of arrival according to (4.26) for a random Gaussian wave packet. This wave packet considered localized (namely its average value for position) to the left of a position X at a time $t = 0$ and which is moving (ie. not zero velocity) towards this X point to the right. In the Heisenberg picture - momentum basis, a state representing a Gaussian wave packet, centered at k_0 and with a width of $1/\delta$, has a normalized expression of the form:

$$\psi(k) = \left(\frac{2\delta^2}{\pi}\right)^{\frac{1}{4}} \exp\left[-(k-k_0)^2\delta^2 - ikx_0\right] \tag{4.27}$$

Substituting this wave packet expression inside (4.26) and calculating the integral gives a long-winded result for the probability distribution equation. Preforming then a series of approximations and expansions of small quantities [19, p. 16, 17], the authors managed to reach to a more convenient form of the result, accurate up to an $(1/k_0\delta)$ order:

$$\pi(T;X) = \frac{\hbar}{m\sqrt{2\pi}} \frac{k_0\delta^2 + \frac{(X-x_0)T\hbar}{4m\delta^2}}{\left(\delta^2 + \frac{T^2\hbar^2}{4m^2\delta^2}\right)^{3/2}} \exp\left(-\frac{(X - x_0 - k_0T\hbar/m)^2)}{2\left(\delta^2 + \frac{T^2\hbar^2}{4m^2\delta^2}\right)}\right) \tag{4.28}$$

Finally, this result for the probability distribution of the time of arrival of a wave packet was plotted to a graph [Figure 4.1] (with the time of arrival on the horizontal axis) for various (detector) positions X (mentioned below) with the constants of the expression set to the values of: $x_0 = -5$, $k_0 = 20$, $\delta_0 = 0.5$ and $\hbar = m = 1$:

As expected the distribution is roughly centered on the classical time-of-arrival value, with a left and right (quantum) spread along the T axis. The width of this spread, as we can directly observe on the plot above or from the expression (4.28), increases as the X position moves to the right, ie. as the detector moves further away from the initial location of the wave packet. In other words, while the wave packet evolves from its initial state, its width spreads more due to the fact that the different parts of the wave packet move with a different velocity and thus causing it to spread more in space. Therefore, for further distances of the detector, this property of the wave packet results to a wider interval of detected values for the time-of-arrival quantity, namely a wider, more spread time-of-arrival probability distribution.

4.2 Modyfing both operators

In the second part of this chapter the work of Delgado and Muga from their 1997 paper [12] is presented. According to the researchers, inside this

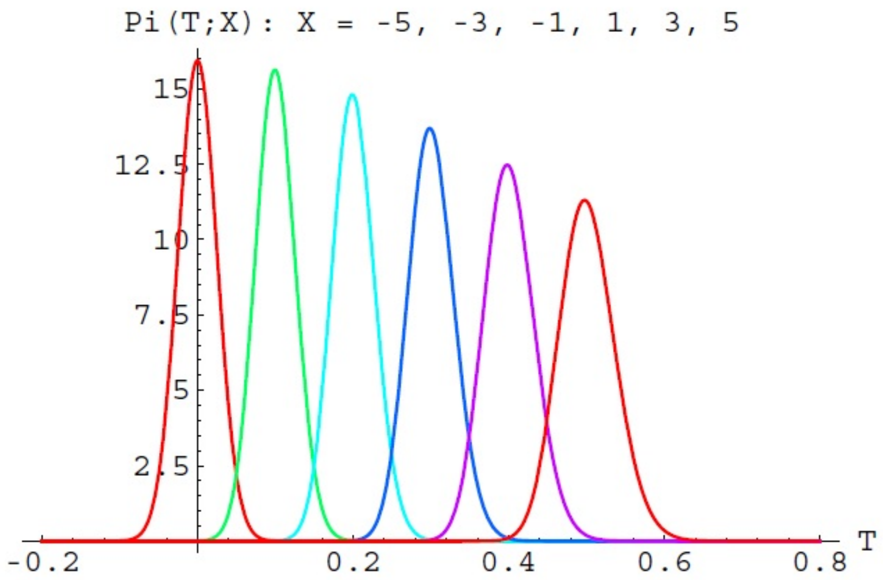

Figure 4.1: Time-of-arrival probability distribution of a Gaussian wave packet

paper an attempt to circumvent Pauli's theorem was made. Instead of expanding only the time-of-arrival operator, while leaving the semi-bounded Hamiltonian as it is, ie. the case of the previous part, Delgado and Muga introduce a new hypothetical and convenient operator $\hat{\mathcal{H}}$ with dimensions of energy, defined this time in the whole spectrum of energy, negative and positive. Correspondingly then, a new self-adjoint operator of dimensions of time conjugated to this new energy operator is defined, which is used to reach to the desired expression of the time-of-arrival probability distribution for the free particle case (again no degrees of freedom from detectors were assumed).

4.2.1 Introducing a new commutation relation

It was proven in detail in Chapter 2 (3.1) that a commutation relation $[\hat{H}, \hat{T}] = i\hbar$, for the Hamiltonian and a time operator, is not consistent with the semi-bounded character of the energy spectrum of the Hamiltonian. It's tempting though to investigate the hypothetical case that the Hamiltonian operator is not bounded, but rather defined in the whole energy spectrum. Of course, this change of the domain of the Hamiltonian will transform the operator to a new one; we can't assume that we refer to the physical Hamiltonian anymore. It will be a new self-adjoint operator with dimensions of energy $\hat{\mathcal{H}}$.

Furthermore, building to our assumptions, if we postulate that there's another conjugated operator to this new energy operator, $\hat{\mathcal{T}}$, it's reasonable to except that this conjugated operator will have the dimensions of time. Of course, no prior association with the physical time can be assumed. However, if we still postulate that the new energy operator and its conjugate have exactly the same domains of definition, then it is valid to introduce a commutation relation for these two operators, like the one forbidden by Pauli's "Theorem":

$$[\hat{\mathcal{H}}, \hat{\mathcal{T}}] = i\hbar\,. \tag{4.29}$$

where we cannot yet consider both of the operators involved as self-adjoint, only $\hat{\mathcal{H}}$ (see for further below (4.2.3)).

The authors admit that indeed these assumptions are in a sense arbitrary, but still quite reasonable though. The whole attempt aims to the construction of a proper self-adjoint operator $\hat{\mathcal{T}}$ with dimensions of time, which operator will be associated carefully with the classical quantity of time of arrival in order to reach to an expression for the probability distribution of the time of arrival.

4.2.2 Non-bounded energy states and a new energy operator

The experimental case in consideration is again the simple one-dimensional free particle case, described in detail in Chapter 2 (see (**??**)). The free Hamiltonian is $H_0 = \hat{P}^2/2m$ and even its energy spectrum is bounded, its momentum spectrum is not, negative momenta belong to its support. Specifically, the energy spectrum in the free case is degenerate to the momentum values, ie. for each energy value correspond two momenta of opposite sign: $p = \pm\sqrt{2mE}$. Thus, rewriting the eigenvalue equation for the momentum operator, by denoting the momentum eigenstates with their corresponding energy value:

$$\begin{gathered} \hat{P}\,|p\rangle = p\,|p\rangle \\ \Rightarrow \hat{P}\,|E\rangle = \pm\sqrt{2mE}\,|E\rangle \ , \end{gathered}$$

Hence, it is made obvious that the energy eigenstates can be also (after proper normalization) eigenstates of the momentum operator, despite their degeneracy.

For notational purposes, we can denote this momentum eigenstates, attributed by the energy value, with the additional information of the sign of the momenta values, schematically in the following 1:1 correspondence:

$$|p\rangle \to |E; \mathrm{sgn}\,(p)\rangle \equiv |E; \pm\rangle \ ,$$

which states of course are still energy eigenstates:

$$\hat{H}_0 \, |E; \pm\rangle = E \, |E; \pm\rangle \ , \tag{4.30}$$

However, unlike the standard energy eigenstates, these states form a complete set of states because their spectrum is not confined to the half of the energy axis as with the semi-bounded spectrum of the Hamiltonian. They are defined through the whole axis. Their completeness is a direct consequence of the completeness relation for the momentum eigenstates, after a proper normalization. Let $|p\rangle \equiv A \, |E; \pm\rangle$. From the classical-free-case relation:

$$p^2 = 2mE \Rightarrow |p| \, dp = m \, dE \, ,$$

the completeness relation for the momentum eigenstates turns into:

$$\int_{-\infty}^{\infty} dp \ |p\rangle \, \langle p| = \hat{1} \tag{4.31}$$

$$\Rightarrow \sum_{a=\mathrm{sgn}\,(p(E))} \int_0^{\infty} dE \frac{m}{|p(E)|} A^2 \, |E; \alpha\rangle \, \langle E; \alpha| = \hat{1}$$

Thus considering then $A \equiv \mathrm{sgn}\,(|p(E)|)\sqrt{|p|/m}$ for the normalization constant, we get the completeness relation for the $\{|E; \alpha\rangle\}$ states:

$$\Rightarrow \sum_{a=\pm} \int_0^{\infty} dE \, |E; \alpha\rangle \, \langle E; \alpha| = \hat{1} \tag{4.32}$$

and the exact relation that associates the states $\{|E; \alpha\rangle\}$ to the momentum eigenstates $\{|p\rangle\}$:

$$|p\rangle = \mathrm{sgn}\,\big(|p|\big)\sqrt{\frac{|p|}{m}} \, |E; \pm\rangle$$

$$\Rightarrow |p\rangle = \pm \left(\frac{2E}{m}\right)^{1/4} |E; \pm\rangle \tag{4.33}$$

Furthermore, these states are orthonormal, a consequence again of the orthogonality of the momentum eigenstates:

$$\langle p|p'\rangle = \delta(p - p')$$

$$\Rightarrow \int_{-\infty}^{\infty} dp \ \langle p|p'\rangle = 1$$

and using (4.33) in replacing the $\{|p\rangle\}$ states:

$$\Leftrightarrow \sum_{a=\pm} \int_0^\infty dE \frac{m}{p(E)} A^2 \langle E;\alpha|E';\alpha'\rangle = 1$$

$$\Rightarrow \sum_{a=\pm} \int_0^\infty dE \langle E;\alpha|E';\alpha'\rangle = 1 \tag{4.34}$$

$$\Rightarrow \langle E;\alpha|E';\alpha'\rangle = \delta_{aa'}\delta(E-E') \tag{4.35}$$

Thus it is proven that we now have indeed a valid, complete and orthonormal set of energy eigenstates: $\{|E;\alpha\rangle\}$.

For convenience another notation is introduced for these states with a parameter ϵ of energy dimensions defined in the whole energy spectrum, ie. $\epsilon \in (-\infty, +\infty)$:

$$|\epsilon\rangle = \begin{cases} |E;+\rangle\,, & \text{if } \epsilon \geq 0 \\ |E;-\rangle\,, & \text{if } \epsilon \leq 0 \end{cases} \tag{4.36}$$

Following from (4.32) and (4.35), a completeness relation and the orthogonality of these $|\epsilon\rangle$ states are straightforward to see:

$$\Rightarrow \int_{-\infty}^{\infty} d\epsilon\, |\epsilon\rangle \langle\epsilon| = \hat{1} \tag{4.37}$$

$$\Rightarrow \langle\epsilon|\epsilon'\rangle = \delta(\epsilon-\epsilon')\,, \tag{4.38}$$

as well as the action of the free Hamiltonian on these states:

$$\hat{H}_0\,|\epsilon\rangle = |\epsilon|\,|\epsilon\rangle\ , \tag{4.39}$$

Hence, a complete and orthogonal set of energy eigenstates attributed by the non-bounded energy parameter ϵ has been obtained, $\{|\epsilon\rangle\}$. It was a carefully defined procedure and Delgado and Muga make another step defining carefully again an operator of energy dimensions $\hat{\mathcal{H}}$, with non-bounded support in terms of the ϵ parameter, for which also these $\{|\epsilon\rangle\}$ states will be its eigenstates, namely:

$$\hat{\mathcal{H}}\,|\epsilon\rangle = \epsilon\,|\epsilon\rangle\ . \tag{4.40}$$

or from the definition of the $\{|\epsilon\rangle\}$ states (4.36):

$$\hat{\mathcal{H}}\,|E;\pm\rangle = \pm E\,|E;\pm\rangle$$

Thus the action of this $\hat{\mathcal{H}}$ operator can be roughly described as being identical with that of the free Hamiltonian $\hat{H}_0$ for states of positive ϵ value and for states of negative ϵ value is almost identical, with the difference that it assigns to the corresponding $|\epsilon|$ energy eigenstate a minus sign.

In order then for Delgato and Muga to "rephrase" this action of the $\hat{\mathcal{H}}$ operator in terms of operators and domains of definition, they suggest that the action of $\hat{\mathcal{H}}$ is consisted by the consecutive actions of two operators, the free Hamiltonian operator $\hat{H}_0$, on the one hand, and a proper sign operator, on the other. Thus the definition of a sign operator is necessary. The following aside describes in detail the construction of this sign operator needed for extracting the sign of the ϵ parameter in the $\{|\epsilon\rangle\}$ states.

The sign operator

Rewriting for start (4.33) as follow:

$$|p\rangle = \alpha\sqrt{\frac{|p|}{m}}\,|E;\alpha\rangle \ ,\alpha = \mathrm{sgn}\,(p(E))$$

and projecting then an energy eigenstate on a momentum eigenstate, using also the orthogonality relation (4.35), we get:

$$\Rightarrow \langle p|E';\alpha'\rangle = \alpha\sqrt{\frac{|p|}{m}}\,\langle E;\alpha|E';\alpha'\rangle = \alpha\sqrt{\frac{|p|}{m}}\,\delta_{aa'}\delta(E-E')\,.$$

We notice the sign-of-the-momentum variable α appears as a factor inside the last expression along with the others. This indicates a procedure for which the sign of the momenta becomes significant. Multiplying then $\langle p|E';\alpha'\rangle$ to another momentum eigenstate (the conjugate to $\langle p|$) and rewriting it as an energy eigenstate:

$$\Rightarrow \langle p|E';\alpha'\rangle\,|p\rangle = \left(\alpha\sqrt{\frac{|p|}{m}}\,\delta_{aa'}\delta(E-E')\right)\alpha\sqrt{|p|/m}\,|E;\alpha\rangle$$
$$= \alpha^2\frac{|p|}{m}\,\delta_{aa'}\delta(E-E')\,|E;\alpha\rangle$$

Of course the α^2 term equals now to 1. And since $dE = |p|\,dp/m$, integrating the whole expression for momentum values only on the halve of the momenta values axis, since we refer to a specific value for α (let's assume $\alpha = +$) we get:

$$\Rightarrow \int_0^\infty dp\,|p|/m\,\delta_{(+)a'}\delta(E-E')\,|E;+\rangle$$
$$= \int_0^\infty dE\,\delta_{(+)a'}\delta(E-E')\,|E;+\rangle = \delta_{(+)a'}\,|E';+\rangle\ .$$

Integrating this time over half of the axis of a variable for the Kronecker delta function is valid, since E is not defined on the whole axis and we can consider that, for these negative values, the ket $|E';+\rangle$ is simply the zero vector.

$$\Rightarrow \delta_{(+)a'}\,|E';+\rangle = \begin{cases} |E;+\rangle\,, & \text{if } \alpha' = + \\ 0\,, & \text{if } \alpha' = - \end{cases} \tag{4.41}$$

Hence, the result of this whole aforementioned procedure is eventually the initial energy eigenstate, if it had positive momenta and it's the zero vector (of the Hilbert space), if it had negative momenta. It's no difficult to see that the whole process actually is the action of this projection operator:

$$\int_0^\infty dp\ |p\rangle\,\langle p|$$

on the $|E;\alpha\rangle$ states.

It resembles the completeness relation of the momentum eigenstates (4.31), however the integration range is on the half axis of the momenta values. Furthermore, if we had integrated for the negative momenta values, the result would have been reversed, but without assigning a minus sign to the initial energy eigenstate:

$$\left(\int_{-\infty}^0 dp\,|p\rangle\langle p|\right)|E;\alpha\rangle = \begin{cases} 0\,, & \text{if } \alpha' = + \\ |E;+\rangle\,, & \text{if } \alpha' = - \end{cases} \tag{4.42}$$

Therefore from these two procedures we define the following projection operators:

$$\Theta(\pm\hat{P}) \equiv \int_0^\infty dp\ |\pm p\rangle\,\langle \pm p| \tag{4.43}$$

and if our aim is to construct an operator which reproduces the initial state along with the sign of the momenta, we can define using (4.43) the desired self-adjoint sign operator:

$$\operatorname{sgn}(\hat{P}) \equiv \Theta(\hat{P}) - \Theta(-\hat{P})\,. \tag{4.44}$$

Extending the Hamiltonian

Hence now using (4.44), we can accurately define the $\hat{\mathcal{H}}$ operator in consistency with the aforementioned description:

$$\hat{\mathcal{H}} \equiv \operatorname{sgn}(\hat{P})\hat{H}_0 \tag{4.45}$$

Otherwise, we can consider the free Hamiltonian as the operator defined for a set of states, which states are the projection for only positive ϵ values of these general states defined in the domain of the extended $\hat{\mathcal{H}}$ operator of energy dimensions.

4.2.3 A self-adjoint "time" operator

Summarizing, we have established so far a valid self-adjoint operator with dimensions of energy $\hat{\mathcal{H}}$, along with its complete and orthogonal set of eigenstates $\{|\epsilon\rangle\}$, on the one hand. And on the other hand, a commutation relation for this $\hat{\mathcal{H}}$ operator with a conjugate operator of dimensions of time $\hat{\mathcal{T}}$ has been assumed that it exists (4.29). The next step forward now is to associate this $\hat{\mathcal{T}}$ operator with the actual measured time, if it's possible. And a way through this is to check if $\hat{\mathcal{T}}$ correspond to a hypothetical real value quantity via its eigenvalues (ie. that it's self-adjoint indeed). Then we can check for any relation that links this hypothetical quantity to physical time.

The set $\{|\tau\rangle\}$ of the eigenstates of this $\hat{\mathcal{T}}$ operator are defined by its eigenvalue equation: $\hat{\mathcal{T}}|\tau\rangle = \tau|\tau\rangle$. Completeness and orthogonally for the $\{|\tau\rangle\}$ eigenstates are the two conditions necessary and sufficient for the operator $\hat{\mathcal{T}}$ to be proven self-adjoint. The step-by-step, strict proof of the self-adjointness of the $\hat{\mathcal{T}}$ operator, conjugated to the $\hat{\mathcal{H}}$ operator as this was defined above for the free particle case, follows:

Proof for the self-adjointness of the $\hat{\mathcal{T}}$ operator

The only prior assumptions for this proof is the validity of the commutation relation (4.29) and the defining expression for the $\hat{\mathcal{H}}$ operator (4.45):

1. Firstly let's replace the expression for the $\hat{\mathcal{H}}$ operator from (4.45) inside the commutation relation (4.37):

   $$[\hat{\mathcal{H}}, \hat{\mathcal{T}}] = [\text{sgn}(\hat{P})\hat{H}_0, \hat{\mathcal{T}}] = [\text{sgn}(\hat{P}), \hat{\mathcal{T}}]\hat{H}_0 + \text{sgn}(\hat{P})\,[\hat{H}_0, \hat{\mathcal{T}}] = i\hbar\,,$$

   We have good reasons to make the assumption that the $\text{sgn}(\hat{P})$ and the $\hat{\mathcal{T}}$ operators commute, since we want to associate $\hat{\mathcal{T}}$ with physical time in the free case. The sign of the velocity and of the momenta changes by definition if we assume a reversal of the flow of time, or a time-reversal transformation. Thus the least we can do in order for $\hat{\mathcal{T}}$ to exhibit a similar property under time-reversals (it doesn't guarantee it of course) is to assign to the expansion of the $|\tau\rangle$ states in terms of momentum eigenstates, only a spectrum of momentum eigenstates of the same sign, negative or positive. This is still of course an assumption, mainly for convenience in the calculations and in the interpretation.

   From this last assumption then we are lead to:

   $$[\hat{H}_0, \hat{\mathcal{T}}] = \begin{cases} +i\hbar\,, & \text{for } \epsilon > 0 \\ -i\hbar\,, & \text{for } \epsilon < 0 \end{cases} \tag{4.46}$$

2. This last result (4.46) has significant consequences on the way we can associate the operator $\hat{\mathcal{T}}$ with the actual time. A first investigation of this association (further analysis in (4.2.4)) has to be done following a procedure similar to the one of Chapter 3 (3.1.2), while proving the nonexistence of a self-adjoint time operator conjugated to the Hamiltonian. To begin with, we construct another commutation relation for an exponential, this time, expression of the Hamiltonian, using for start the $\epsilon > 0$ part of (4.46) and the next property of the commutators (given of course that every positive integer power of the free Hamiltonian exists):

$$[\hat{H}_0^n, \hat{\mathcal{T}}] = in\hbar\hat{H}_0^{n-1}, \quad n \geq 1 \tag{4.47}$$

If we then multiple both parts of (4.47) with $(-it/\hbar)^n/n!$, where t is an arbitrary parameter of dimensions of time, and sum over all the powers of n, while taking $(H_0)^0 \equiv \hat{1}$:

$$\begin{aligned} &\Rightarrow [e^{-i\hat{H}_0 t/\hbar}, \hat{\mathcal{T}}] = te^{-i\hat{H}_0 t/\hbar} \\ &\Rightarrow \hat{\mathcal{T}} e^{-i\hat{H}_0 t/\hbar} |\tau\rangle = (\tau - t)e^{-i\hat{H}_0 t/\hbar} |\tau\rangle \\ &\Rightarrow e^{-i\hat{H}_0 t/\hbar} |\tau\rangle = |\tau - t\rangle \end{aligned} \tag{4.48}$$

The corresponding result for $\epsilon < 0$ from (4.46) is:

$$\Rightarrow e^{-i\hat{H}_0 t/\hbar} |\tau\rangle = |\tau + t\rangle \tag{4.49}$$

Since we refer to the free Hamiltonian operator $\hat{H}_0$, this exponential function $e^{-i\hat{H}_0 t/\hbar}$ can be considered as the time evolution operator, if t is postulated to be a parameter for the actual time. And what we can infer then from (4.48) and (4.49) is that the behaviour of the eigenstates of this $\hat{\mathcal{T}}$ operator on time evolution is different for positive momenta values ($\epsilon > 0$) and different for negative momenta values ($\epsilon < 0$). For positive momenta the τ parameter decreases with the time passing, while for negative momenta τ increases. Further remarks on the association of t and τ in (4.2.4).

3. Next we investigate the expression for $\langle\tau|\epsilon\rangle$, ie. the projection of an eigenstate of the $\hat{\mathcal{H}}$ operator to an eigenstate of the $\hat{\mathcal{T}}$ operator. An exponential expression of the form: $\exp(-i\epsilon\tau/\hbar)$ is expected, mainly from its similarity with: $\exp(-i\hat{H}_0 t/\hbar)|E\rangle = \exp(-i\hat{E}t/\hbar)|E\rangle$. Rewriting first the eigenvalue equation of $\hat{\mathcal{H}}$ (4.40) using (4.39) and (4.45) we get:

$$\hat{\mathcal{H}} |\epsilon\rangle = \mathrm{sgn}(\hat{P})\hat{H}_0 |\epsilon\rangle = \mathrm{sgn}(\hat{P})|\epsilon| |\epsilon\rangle \tag{4.50}$$

Thus the time evolution of the $\{|\epsilon\rangle\}$ states from (4.50) is:

$$\exp\left(-i\hat{H}_0 t/\hbar\right)|\epsilon\rangle = \exp\left(-i|\epsilon|t/\hbar\right)|\epsilon\rangle \tag{4.51}$$

Projecting then (4.51) on an eigenstate of $\hat{\mathcal{T}}$:

$$\begin{aligned} &\Rightarrow \langle\tau|\exp\left(-i\hat{H}_0 t/\hbar\right)|\epsilon\rangle = \langle\tau|\exp\left(-i|\epsilon|t/\hbar\right)|\epsilon\rangle \\ &\Leftrightarrow \langle\tau|\exp\left(-i\hat{H}_0 t/\hbar\right)|\epsilon\rangle = \exp\left(-i|\epsilon|t/\hbar\right)\langle\tau|\epsilon\rangle \end{aligned} \tag{4.52}$$

It will be now useful to calculate the action of the time evolution operator on the bra: $\langle\tau|$. It corresponds of course to the action of the adjoint of the time evolution operator: $(\exp\left(-i\hat{H}_0 t/\hbar\right))^\dagger = \exp\left(i\hat{H}_0 t/\hbar\right)$ on the ket: $|\tau\rangle$. So, in order to use (4.48) and (4.49) immediately, we have to consider another parameter instead of t of opposite sign, say $t \equiv -t'$ and then (4.48) and (4.49) turn into:

$$\exp\left(i\hat{H}_0 t'/\hbar\right)|\tau\rangle = \begin{cases} |\tau + t'\rangle \ , & \epsilon > 0 \\ |\tau - t'\rangle \ , & \epsilon < 0 \end{cases} \tag{4.53}$$

Therefore, we can infer from (4.52) and (4.53) that:

$$\langle\tau|\exp\left(-i\hat{H}_0 t/\hbar\right)|\epsilon\rangle = \begin{cases} \langle\tau + t|\epsilon\rangle = \exp\left(-i|\epsilon|t/\hbar\right)\langle\tau|\epsilon\rangle \ , & \epsilon > 0 \\ \langle\tau - t|\epsilon\rangle = \exp\left(-i|\epsilon|t/\hbar\right)\langle\tau|\epsilon\rangle \ , & \epsilon < 0 \end{cases} \tag{4.54}$$

Applying then a simple trick in order to avoid t dependence, we set the $\langle\tau \pm t|\epsilon\rangle$ scalar products as $\langle 0|\epsilon\rangle$, ie. $t \equiv \mp\tau$ correspondingly for positive and negative momenta:

$$\begin{aligned} &\Rightarrow \langle 0|\epsilon\rangle = \exp\left[-i|\epsilon|(\mp\tau)/\hbar\right]\langle\tau|\epsilon\rangle \\ &\Leftrightarrow \langle\tau|\epsilon\rangle = \langle 0|\epsilon\rangle \exp\left[i|\epsilon|(\mp\tau)/\hbar\right] \end{aligned} \tag{4.55}$$

Furthermore, it is more illuminating in (4.55) to write the absolute value of ϵ as $\pm\epsilon$:

$$\begin{aligned} &\Rightarrow \langle\tau|\epsilon\rangle = \langle 0|\epsilon\rangle \exp\left[i(\pm\epsilon)(\mp\tau)/\hbar\right] \\ &\Rightarrow \langle\tau|\epsilon\rangle = \langle 0|\epsilon\rangle \exp\left(-i\epsilon\tau/\hbar\right) \end{aligned} \tag{4.56}$$

Hence, indeed a general expression for $\langle\tau|\epsilon\rangle$ can be obtained, valid for both cases of momenta sign. The $\langle 0|\epsilon\rangle$ scalar product in (4.56) can be considered as the normalization factor of the equation dependent only on the value of the ϵ parameter.

4. In order to specify the exact expression for $\langle 0|\epsilon\rangle$, we repeat carefully the procedure of point 1, but with powers of the $\hat{\mathcal{T}}$ operator this time, multiplying it with a factor of $(-iE/\hbar)^n/n!$, with E an arbitrary parameter of dimensions of energy $((\hat{\mathcal{T}}_0)^0 \equiv \hat{1})$:

$$\begin{aligned}
[\hat{H}_0, \hat{\mathcal{T}}^n] &= \pm i n\hbar \hat{\mathcal{T}}_0^{n-1}, \quad (n \geq 1) \\
\Rightarrow [\hat{H}_0, \frac{(-i\hat{\mathcal{T}}E/\hbar)^n}{n!}] &= \pm E \frac{(-i\hat{\mathcal{T}}E/\hbar)^{n-1}}{(n-1)!} \\
\Rightarrow [\hat{H}_0, e^{-i\hat{\mathcal{T}}E/\hbar}] &= \pm E e^{-i\hat{\mathcal{T}}E/\hbar} \\
\Rightarrow \hat{H}_0\, e^{-i\hat{\mathcal{T}}E/\hbar}|\epsilon\rangle - e^{-i\hat{\mathcal{T}}E/\hbar}\, \hat{H}_0|\epsilon\rangle &= \pm E\, e^{-i\hat{\mathcal{T}}E/\hbar}|\epsilon\rangle \\
\Rightarrow \hat{H}_0\, e^{-i\hat{\mathcal{T}}E/\hbar}|\epsilon\rangle &= (|\epsilon| \pm E)\, e^{-i\hat{\mathcal{T}}E/\hbar}|\epsilon\rangle \\
\Rightarrow e^{i\hat{\mathcal{T}}E/\hbar}|\epsilon\rangle &= ||\epsilon| \pm E\rangle \qquad (4.57)
\end{aligned}$$

The action of the $e^{i\hat{\mathcal{T}}E/\hbar}$ operator on a bra $\langle\epsilon|$ is:

$$\Rightarrow \langle\epsilon|e^{-i\hat{\mathcal{T}}E/\hbar} = \langle|\epsilon| \mp E|\,, \qquad (4.58)$$

Projecting then on a ket $|\tau\rangle$:

$$\Rightarrow \langle\epsilon|e^{i\hat{\mathcal{T}}E/\hbar}|\tau\rangle = e^{-i\tau E/\hbar}\langle\epsilon|\tau\rangle = \langle|\epsilon| \mp E|\tau\rangle \qquad (4.59)$$

and therefore by setting $E = \pm|\epsilon|$:

$$\Rightarrow \langle\epsilon|\tau\rangle = \langle 0|\tau\rangle e^{i\tau E/\hbar}\,. \qquad (4.60)$$

If we seek to calculate $\langle 0|\epsilon\rangle$ from (4.60), which is the complex conjugate of (4.56), we observe that:

$$\Rightarrow \langle\epsilon|0\rangle = \langle\epsilon = 0\,|\tau = 0\rangle\,. \qquad (4.61)$$

Hence, the normalization factor $\langle 0|\epsilon\rangle$ is independent from the ϵ parameter too, eventually it's a constant and we will denote it as A. In conclusion, the exact expression for the scalar product $\langle\tau|\epsilon\rangle$ is:

$$\langle\tau|\epsilon\rangle = A\, e^{-i\epsilon\tau/\hbar} \qquad (4.62)$$

and for its complex conjugate from (4.60):

$$\langle\epsilon|\tau\rangle = \bar{A}\, e^{i\epsilon\tau/\hbar}\,, \qquad (4.63)$$

where we have to observe that we used τ and not its complex conjugate (we never assumed τ to be real). Thus, τ is definitely real, another indication (not proof) that we' re dealing with a self-adjoint operator.

5. Next let's check if the $\{|\tau\rangle\}$ states are orthonormal, using the completeness relation for the $\{|\epsilon\rangle\}$ states (4.37) and the equations (4.62) and (4.63):

$$\langle\tau|\tau'\rangle = \int_{-\infty}^{\infty} d\epsilon\, \langle\tau|\epsilon\rangle\, \langle\epsilon|\tau'\rangle = |A|^2 \int_{-\infty}^{\infty} d\epsilon\, e^{-i\epsilon(\tau-\tau')/\hbar}$$
$$= |A|^2 2\pi\hbar\delta(\tau-\tau') = |A|^2 h\delta(\tau-\tau')$$

So imposing for the normalization constant a value of $|A| = h^{-1/2}$ we get the exact expression for $\langle\tau|\epsilon\rangle$:

$$\langle\tau|\epsilon\rangle = h^{-1/2}\, e^{-i\epsilon\tau/\hbar}, \tag{4.64}$$

and also we get a proper orthogonality relation for the $\{|\tau\rangle\}$ eigenstates:

$$\langle\tau|\tau'\rangle = \delta(\tau-\tau') \tag{4.65}$$

6. Last of the steps is proving the completeness for the $\{|\tau\rangle\}$ eigenstates. For start let's expand a $|\tau\rangle$ eigenstate in terms of the $\{|\epsilon\rangle\}$ states using again (4.37) and (4.64):

$$|\tau\rangle = \hat{1}\,|\tau\rangle = \left(\int_{-\infty}^{\infty} d\epsilon\, |\epsilon\rangle\, \langle\epsilon|\right)|\tau\rangle = \int_{-\infty}^{\infty} d\epsilon\, \langle\epsilon|\tau\rangle\, |\epsilon\rangle$$
$$\Rightarrow |\tau\rangle = h^{-1/2} \int_{-\infty}^{\infty} d\epsilon\, e^{i\epsilon\tau/\hbar}\, |\epsilon\rangle \tag{4.66}$$

So substituting (4.66) inside the expression under investigation:

$$\int_{-\infty}^{\infty} d\tau\, |\tau\rangle\, \langle\tau| = h^{-1} \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\epsilon\, e^{i\epsilon\tau/\hbar}\, |\epsilon\rangle \int_{-\infty}^{\infty} d\epsilon'\, e^{-i\epsilon'\tau/\hbar}\, \langle\epsilon'|$$
$$= h^{-1} \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\epsilon'\, e^{i(\epsilon-\epsilon')\tau/\hbar}\, |\epsilon\rangle\, \langle\epsilon'|$$
$$= h^{-1} \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\epsilon' \int_{-\infty}^{\infty} d\tau\, e^{i(\epsilon-\epsilon')\tau/\hbar}\, |\epsilon\rangle\, \langle\epsilon'|$$
$$= \frac{2\pi\hbar}{h} \int_{-\infty}^{\infty} d\epsilon \int_{-\infty}^{\infty} d\epsilon'\, \delta(\epsilon-\epsilon')\, |\epsilon\rangle\, \langle\epsilon'|$$
$$= \int_{-\infty}^{\infty} d\epsilon\, |\epsilon\rangle\, \langle\epsilon| = \hat{1}$$

Hence the completeness relation for the $\{|\tau\rangle\}$ states is also proven:

$$\int_{-\infty}^{\infty} d\tau\, |\tau\rangle\, \langle\tau| = \hat{1}\,. \tag{4.67}$$

Conclusively, we painstakingly managed to prove rigorously the self-adjointness of this $\hat{\mathcal{T}}$ operator we defined. Indeed for the free particle case, extending the Hamiltonian to a new expanded operator $\hat{\mathcal{H}}$ of energy dimensions and assuming a conjugate operator $\hat{\mathcal{T}}$, defined on the same exact domain with $\hat{\mathcal{H}}$, of dimensions of time, with the additional assumption that $\hat{\mathcal{T}}$ commutes with the $\text{sgn}(\hat{P})$ operator, it results to the self-adjointness of $\hat{\mathcal{T}}$, unlike with case of the Hamiltonian and an any-way-defined time operator.

An expression for the $\hat{\mathcal{T}}$ operator

Moreover, provided now the orthogonal and complete set of eigenstates $\{|\tau\rangle\}$ of the $\hat{\mathcal{T}}$ operator, an expression of this operator can be constructed from its spectral decomposition using relation (4.6) from the previous part of the chapter:

$$\hat{\mathcal{T}} = \int_{-\infty}^{\infty} d\tau\, \tau\, |\tau\rangle \langle\tau| \tag{4.68}$$

.

4.2.4 Association with physical time

Defining a self-adjoint operator with dimensions of time conjugated to this extended "energy" operator is of course a great step, however it's still not so clear how useful it can be for the definition of a time-of-arrival operator or simply for the derivation of a probability distribution for the time of arrival.

Having in mind these objectives, an immediate and reasonable question is if the $\hat{\mathcal{T}}$ operator can be identified as the operator for the actual physical time that our defectors measure. The answer is negative. One way to see this is from (4.48) and (4.49). The $\{|\tau\rangle\}$ states behave differently in time evolution for positive and differently for negative: the τ parameter decreases in an evolution in time for positive momenta and decreases for negative. And even if we are tempted to confine ourselves using only for example positive momenta and using the τ parameter in a way to indicates time (using the opposite of the τ parameter for example), Delgado and Muda [12, p. 8] discourage us even more while mentioning that the $\{|\tau\rangle\}$ states are invariant under time reversal, something unacceptable for states corresponding to measurements of the actual physical time.

So eventually, how is the $\hat{\mathcal{T}}$ operator associated with the physical time, according to Delgado and Muga? Contemplating on (4.66), we can observe a way we can bring about physical time in our equations by splitting this spectral decomposition into contributions from negative momenta values and positive momenta values and bringing back the momenta sign notation $|E;\pm\rangle$ for the $|\epsilon\rangle$ states:

$$
\begin{aligned}
|\tau\rangle &= h^{-1/2}\int_{-\infty}^{0} d\epsilon\, e^{i\epsilon\tau/\hbar}\,|\epsilon\rangle + h^{-1/2}\int_{0}^{\infty} d\epsilon\, e^{i\epsilon\tau/\hbar}\,|\epsilon\rangle \\
&= -h^{-1/2}\int_{\infty}^{0} dE\, e^{-iE\tau/\hbar}\,|E;-\rangle + h^{-1/2}\int_{0}^{\infty} dE\, e^{iE\tau/\hbar}\,|E;+\rangle \\
&= h^{-1/2}\int_{0}^{\infty} dE\, e^{-iE\tau/\hbar}\,|E;-\rangle + h^{-1/2}\int_{0}^{\infty} dE\, e^{iE\tau/\hbar}\,|E;+\rangle \ . \qquad (4.69)
\end{aligned}
$$

Let's define then:

$$
|t;\pm\rangle = h^{-1/2}\int_{0}^{\infty} dE\, e^{iEt/\hbar}\,|E;\pm\rangle \ , \qquad (4.70)
$$

with t for the time being just a parameter of time dimensions. So rewriting (4.69) using (4.70) we get:

$$
\Rightarrow |\tau\rangle = |t=-\tau;-\rangle + |t=+\tau;+\rangle \qquad (4.71)
$$

We will then use the expressions (4.48) and (4.49) of the behaviour of the $\{|\tau\rangle\}$ states on the action of the time evolution operator, in order to clarify how this t parameter can be linked with the physical time.

$$
e^{-i\hat{H}_0 t_0/\hbar}\,|\tau\rangle = \begin{cases} e^{i\hat{H}_0 t_0/\hbar}\,|t=-\tau;+\rangle = |\tau-t_0\rangle = |t=+\tau-t_0;+\rangle \ , & \text{for } \epsilon>0 \\ e^{i\hat{H}_0 t_0/\hbar}\,|t=+\tau;-\rangle = |\tau+t_0\rangle = |t=-\tau-t_0;+\rangle \ , & \text{for } \epsilon<0 \end{cases}
$$

So even though the $\{|\tau\rangle\}$ states behave abnormally on time translations, these $\{|t;\pm\rangle\}$ states satisfy (for both momenta signs) a proper time-translation property, namely in time evolution their parameter t is translated by this amount of time for which the evolution operator is defined:

$$
e^{i\hat{H}_0\tau'/\hbar}\,|t;\pm\rangle = |t+\tau';\pm\rangle \qquad (4.72)
$$

However the crucial check will be on how these states behave on time-reversal transformations (as $\{|\tau\rangle\}$ states were checked and failed to be consistent). Let's define for this the $\hat{\mathcal{R}}$ operator as the time-reversal operator. We refer of course to the reversal of sign for the actual time and not necessarily for the t parameter. We investigate thus the action of $\hat{\mathcal{R}}$ on a $|t;\pm\rangle$ state. Since time reversal changes the sign of the momentum value (reversing the flow of time, changes the sign for velocity and thus for momentum) and then $\pm$ turns to $\mp$. Hence from (4.70), t also has to change sign in the $|t;\pm\rangle$ state, in order for the $|\tau\rangle$ state to remain invariant under this transformation (the vary latter about this invariance of $\{|\tau\rangle\}$ is proven in detail by the authors):

$$\hat{\mathcal{R}}\,|t;\pm\rangle = |-t;\mp\rangle \tag{4.73}$$

Hence it is valid now to consider this t parameter as the time parameter of the Schrödinger equation and these $|t;\pm\rangle$ states as eigenstates of a certain time operator. Despite of this success, Delgado and Muga also mention [12, p. 9] that, even though (due to (4.67)) these states are a complete set of states, sadly, they are not orthogonal, a fact that prohibits us from constructing a self-adjoint operator for time measurements of the form (4.6), as we did for the $\hat{\mathcal{T}}$ operator.

4.2.5 The time-of-arrival probability distribution

Following the standard procedure for constructing probability distribution for a measured quantity in quantum mechanics, if these $\{|t;\pm\rangle\}$ states were orthogonal too, since they form a complete set of states, then reaching to an expression for the time-of-arrival probability distribution would have been straightforward. However, they are not, while the $\{|\tau\rangle\}$ states are.

The idea for circumventing this obstacle came for the authors from the decomposition (4.71) of a $|\tau\rangle$ state. Since the $\{|\tau\rangle\}$ states are orthogonal and a complete set, then the same will be valid for functions derived from the scalar product $\langle\tau|\psi\rangle \equiv \psi(\tau)$, $|\psi\rangle$ states in the Heisenberg picture, where ψ are states defined on the whole expanded Hilbert space of the $\hat{\mathcal{H}}$ operator. But what if the spectral decomposition of these $|\psi\rangle$ states is exclusively consisted of momenta eigenstates (ie. well defined momentum) of the same sign? Or in other words, what if we consider for the $|\psi\rangle$ states, only superpositions of plane waves of either negative or positive momentum, but not both? Then immediately:

$$\langle\tau|\psi\rangle = \begin{cases} \langle t;+|\psi\rangle\,, & \text{for } p>0 \\ \langle t;-|\psi\rangle\,, & \text{for } p<0 \end{cases} \tag{4.74}$$

with the orthogonality and the completeness of these states still valid. Hence, it seems that now we acquired specific cases that the use of the these $\{|t;\pm\rangle\}$ states, attributed by the time parameter t, is perfectly acceptable and valid for constructing the probability amplitude and the probability distribution.

For this purpose the authors define the initial setting of the situation under investigation with a wave packet $|\psi(t=0)\rangle$, the ingoing asymptote of which has well-defined momenta values of only positive (or negative) direction. In other words $|\psi(t=0)\rangle = |\psi_{\pm,in}\rangle$ and the action of the operator (4.43) on these states is: $\Theta(\pm\hat{P})\,|\psi(t=0)\rangle = \Theta(\pm\hat{P})\,|\psi_{\pm,in}\rangle = |\psi_{\pm,in}\rangle$, because of course of the fact that these states are a superposition of plane wave states of momenta values of the same sign (direction). For further careful remarks on the initial conditions of the states see (4.1.2).

Also, since we consider the free (quantum) particle case, with the free Hamiltonian: $\hat{H}_0 = \hat{P}^2/2m$, and since the $\Theta(\pm\hat{P})$ operator is by definition a projector operator of momentum eigenstates (integrated over a certain interval), then the $\hat{H}_0$ and the $\Theta(\pm\hat{P})$ operators do commute. Therefore $\Theta(\pm\hat{P})$ and the time-evolution operator $exp(-i\hat{H}_0 t/\hbar)$ commute too. This leads us to infer for the evolved initial state $|\psi(t=0)\rangle$ that:

$$\Theta(\pm\hat{P})\,|\psi_\pm(t)\rangle = |\psi_\pm(t)\rangle \ ,$$

ie. that still for the evolved states too, they are a superposition of plane wave sates of momenta of the same sign as in the initial state. Evolution in time does not change this attribute of the states.

Hence, since the condition for only positive (or negative) momenta is satisfied for these states defined for the free particle case, we can apply the conditional relation (4.74) for the time-of-arrival probability amplitude, with $|\psi\rangle$ states defined to be: $|\psi\rangle = |\psi(t=0)\rangle = |\psi_{\pm,in}\rangle$ (Heisenberg picture).

For convenience we express the $|t;+\rangle$ states in the (4.70) expansion on $|E;\pm\rangle$ states and thus the amplitude (4.74) turns to:

$$\langle t;\pm|\psi\rangle = h^{-1/2}\int_0^\infty dE\, e^{-iEt/\hbar}\langle E;\pm|\psi\rangle \tag{4.75}$$

For later comparison purposes we will express (4.75) in the momentum representation using (4.33), the relation between the energy and momentum eigenstates, ie. $|E;\pm\rangle = \mathrm{sgn}\,(|p|)\sqrt{m/|p|}\,|p\rangle$ and since $dE = |p|\,dp/m$:

$$\langle t;\pm|\psi\rangle = \begin{cases} h^{-1/2}\int_0^\infty dp\,\left(\frac{|p|}{m}\right)\, e^{-ip^2t/2m\hbar}\sqrt{\frac{m}{|p|}}\langle p|\psi\rangle\,, & \text{for } p>0 \\ -h^{-1/2}\int_{-\infty}^0 dp\,\left(\frac{|p|}{m}\right)\, e^{-ip^2t/2m\hbar}\sqrt{\frac{m}{|p|}}\langle p|\psi\rangle\,, & \text{for } p<0 \end{cases}$$

$$\Rightarrow \langle t;\pm|\psi\rangle = \frac{1}{\sqrt{hm}}\int_0^{\pm\infty} dp\sqrt{|p|}\, e^{-ip^2t/2m\hbar}\psi(p) \tag{4.76}$$

Furthermore, we will pursue an expression of (4.78) as a function of k, $p=\hbar k$. Firstly we have to determine the normalization factor between the $|p\rangle$ and the $|k\rangle$ states. It's straightforward if we recall that they are both complete sets of states:

$$\int_{-\infty}^\infty dp\ |p\rangle\,\langle p| = \hat{1} \qquad \text{and} \qquad \int_{-\infty}^\infty dk\ |k\rangle\,\langle k| = \hat{1}\,.$$

Thus using the $p = \hbar k$ relation:

$$\Rightarrow \int_{-\infty}^{\infty} dp\ |p\rangle\langle p| = \hbar \int_{-\infty}^{\infty} dk\ |p\rangle\langle p| = \hat{1}\,,$$

it becomes obvious that we can consider $\hbar^{-1/2}$ as the normalization factor for the relation of the two sets of states, namely:

$$|p\rangle = \frac{1}{\sqrt{\hbar}}|k\rangle \tag{4.77}$$

Therefore we can finally reach to an expression for the amplitude $\langle t;\pm|\psi\rangle$ as a function of k:

$$\Rightarrow \langle t;\pm|\psi\rangle = \sqrt{\frac{\hbar}{2\pi m}} \int_0^{\pm\infty} dk \sqrt{|k|}\, e^{-i\hbar k^2 t/2m} \psi(k) \tag{4.78}$$

This is the probability amplitude for detecting the particle at the origin (since there's not any reference to position). If we want change the detecting position, we have to perform a spatial transformation on the x-axis, or in other words, we have to act on the $|t;\pm\rangle$ states with the unitary operator for spatial translation, as we did in (4.24), in the previous part of the chapter:

$$|t;\pm;X\rangle \equiv e^{-i\hat{P}X/\hbar}|t;\pm\rangle \tag{4.79}$$

Hence, following the same procedure as before, but for the $\langle t;\pm;X|\psi\rangle$ amplitude this time, (4.78) turns into:

$$\Rightarrow \langle t;\pm;X|\psi\rangle = \sqrt{\frac{\hbar}{2\pi m}} \int_0^{\pm\infty} dk \sqrt{|k|}\, e^{-i(\hbar k^2 t/2m - kX)} \psi(k) \tag{4.80}$$

which leads to the amazing result for the probability distribution $\pi(T) \equiv |\langle t;\pm;X|\psi\rangle|^2$:

$$\boxed{\Rightarrow \pi(T) = \frac{\hbar}{2\pi m} \left| \int_0^{\pm\infty} dk \sqrt{|k|}\, e^{-i(\hbar k^2 t/2m - kX)} \psi(k) \right|^2} \tag{4.81}$$

This is exactly the same as Kijowski's distribution (3.16) and surprisingly exactly the same with result as the one we reached at the end of the previous part of the chapter (4.26), using a totally different method and a different series of arguments (the minus sign in the exponential, due to the modulus, becomes irrelevant of course). Further commentary on the coincidence of the results for the two parts of this chapter will be made in the next chapter.

An aside on how to check the validity of the result using the current flux operator

The actual path the authors took for reaching to the probability amplitude result, was firstly to prove by a detailed series of arguments [12, p. 10-16] that the quantity $|\langle t; \pm; X|\psi\rangle|^2$ could indeed represent the time-of-arrival probability distribution, a fact we took for granted in the beginning of our analysis. The reader should remember that we have only associated $\{|t; \pm; X\rangle\}$ states with the concept of the time, as this appears as a parameter in the Schrödinger equation (or the time-evolution operator). No specific reference was made on association of the $\{|t; \pm; X\rangle\}$ states with the measurement of a quantity corresponding to time of arrival. This is indeed really subtle, however from our point of view, for the "ideal" concept of time of arrival and the free-particle case we are considering, we think that this association was already made when the momenta eigenstates and the momenta sign was linked in a specific way to the $\{|t; \pm; X\rangle\}$ states and the τ parameter.

Necessary or not, the authors considered it worthwhile to prove this association. On the one hand, they proved that the time integral of this quantity over the whole time-axis is equal to 1, an important attribute of the desired time-of-arrival probability distribution:

$$\int_{-\infty}^{\pm\infty} dt|\langle t; \pm; X|\psi\rangle|^2 = \langle\psi_\pm|\psi_\pm\rangle = 1\,.$$

due to a completeness relation [12, p. 9]:

$$\sum_{a=\pm}\int_{-\infty}^{\infty} dt|t; \alpha; X\rangle\langle t; \alpha; X| = \hat{1}$$

immediately deduced by (4.67) (of course orthogonality for these states is not valid).

And on the other hand, through more complicated considerations, using an expression for the current density (probability flux) operator, used also in the past by many other researchers, which leads indeed to the standard expression of the current density in non-relativistic Quantum Mechanics:

$$\hat{J}(X) = \frac{1}{2m}\left(\hat{P}|X\rangle\langle X| + |X\rangle\langle X|\hat{P}\right) \tag{4.82}$$

and the energy eigenstates $\{|E; \pm\rangle\}$ (4.30), through which we were lead to the definition of the $\{|t; \pm\rangle\}$ states, they proved that this $\pi(T)$ quantity, as defined above, eventually appears as a (weight) distribution function inside the expression for the average time-of-arrival value $\langle t_X \rangle$. The significance of the average value expression was discussed in Chapter 2 (2.2.2).

This was then another and stronger indication that the $\Pi(T)$ quantity was suitable for a probability distribution since it appears inside the expression of the first (statistical) moment of the t parameter (provided that this parameter is associated with the time of arrival concept). This average expression was a product of a reasonable, but still arbitrary, substitution of the aforementioned current operator (4.82) to the quantum version of the classical average value relation:

$$\langle t_X \rangle = \frac{\int_{-\infty}^{\pm\infty} dt t J(X,t)}{\int_{-\infty}^{\pm\infty} dt J(X,t)}$$

The authors of course make a specific comment on that the (4.82) operator is not perfectly adequate for the desired purpose due to the fact that the probability current it yields is not positive finite for every spatial position, a phenomenon called "Backflow Effect" [26, 36, 8, 9, 37].

We do not present here analytically the whole procedure of the proof, even though interesting indeed and successful in a sense. For more justification on the use of (4.82) as the current operator, the interested reader is redirected to these works [11, 3, 25].

Chapter 5

Final Remarks and Conclusions

"... there is no single unique time observable, but actually a whole class of time of occurrence observables – one associated with each observable event that could occur."
— M. D. Srinivas, R. Vijayalakshmi (1981) [34]

In this last chapter of conclusive remarks, we would to explain our opinion on two aspects of the subject treated inside this project. On the one hand, we would like to attempt to give an explanation on why the two exhaustively presented aforementioned methods coincide in their final results of a probability distribution for the time-of-arrival quantity. And on the other hand, we would like to set straight away the personal opinion, or intuition, of ours that yes, a quantum time quantity can be considered to be an inherit attribute of a quantum mechanical system, if defined properly. We'll treat each part in no specific order.

5.1 Derivation of the Kijowksi's distribution using general arguments

It is a firm belief of the author of this project that the fact that the final results (4.26) and (4.81) of the two different methods presented in the previous chapter, in terms of the time-of-arrival probability distributions, coincide, and moreover that they coincide with the corresponding Kijowski's distribution (and also the distribution derived for the Aharonov-Bohm operator (3.18) through POVMs), is not a coincidence at all. We will try to sketch our own opinion for the reasons of this coinsidence.

5.1.1 Clarifying remarks on the time-of-arrival quantum quantity

Firstly, a list of clarifying points for the time-of-arrival quantum quantity. Muga and Leavens inside an extensive review on the time-of-arrival topic [28, p. 398 - 400], they considered the two methods described inside this project, which use self-adjoint expressions in order to reach to the desired probability distribution, that they are not of much interest and that in the contrary they are even much restrictive in terms of the allowed states used to construct the probability distribution. Moreover, they consider POVM approach much more general and complete.

Indeed, the theory of POVMs seems to be of many potentials and the consistent way it circumvents Pauli's "Theorem" is of great importance. However, our personal opinion is that the successful or not construction of distributions finally is not the actual goal of this mental exercise. The interpretation is the main goal. And even if the distribution constructed are indeed subject of interpretation and of extraction of physical meaning, this mapping from intervals to positive operators must be given some clear physical meaning, not clear to the author of this project yet. Distributions are simply expression, which must be interpreted. They are not the interpretation.

We are in favor then of more plain and "realistic" interpretations, we tend to deviated from positivistic or constructivistic perceptions on Physics, and thus we hence, we would like to attempt to explain with the plainest of the words the whole process, while trying to clarify the cause of the results of the previous chapter. We will do it in the form of Q&A mainly for convenience.

What do we want to measure?

We intend to measure or express probabilistically the value of this quantity we called time of arrival. There's the simplistic impression sometimes that a postulated conjugation of a time quantity with the Hamiltonian, which is expressed by the commutation relation $[H, T] = i\hbar$ is enough to determine straight away the time-of-arrival quantity. This is definitely a misconception due to classical prejudice [10].

In Classical Mechanics, time intervals do not have any distinct characteristics according to the situation. Time-of-flight for example can be identified by a time-of-arrival measurement. However, this is not the case in Quantum Mechanics. More specifically, it must have been already clear to reader that a definition for the time-of-arrival quantity needs certainly the position of arrival. It's not redundant information for reasons of simplicity; it's part of the definition, ie. it's part of the question we are looking for an answer. In other kind of measurements may have been redundant, as in a time-of-flight measurement, the exact spatial limits between which the particle moves are not really necessary. The same for a measurement of when a particle crosses a potential barrier.

That's the reason we are in a significant degree agreed with opinion of Srinivas and Vijayalakshmi stated in the epigraph, that " there is no single unique time observable" [34]. This is a characteristic of the Classical Mechanics not accurate in the Quantum level. And also that's why disagree with the opinion stated by Grot et al. [19, p. 2], that the study of the time-of-arrival problem will contribute to studies of simulations of rates for chemical reactions. Since a chemical reaction does not refer to a specific position and the position too is treated probabilistically, the problem refers to some other quantum time quantity. Maybe a more definite answer on the time-of-arrival problem will clarify much in general on the time measurements, but for the purposes for example of simulating chemical reactions' rates is not specifically adequate as a quantity.

What do we mean by specific position of arrival?

We mean that the ideally that the state measured (while measuring the time of arrival) must be an eigenstate of the position operator at the specific position X. Maybe this sounds not feasible, but this is the definition, this is what we're looking for. By this we do not mean that we perform any measurement of position. This would have destroyed any possibility of measuring an attribute of the system. Simply that the state measure is the eigenstate of position with its spatial parameter equal to X.

Can we measure position and time simultaneously?

No, it will show some kind of proof for it. Let's assume a proper and desired time-of-arrival operator T, conjugated to the Hamiltonian, ie. $[\hat{H}, \hat{T}] = i\hbar$ and then let's consider the Jacobi identity of H, T and X:

$$[[\hat{H}, \hat{T}], \hat{X}] + [[\hat{T}, \hat{X}], \hat{H}] + [[\hat{X}, \hat{H}], \hat{T}] = 0$$

Due to the postulated commutation relation, the first term is zero:

$$\Rightarrow [[\hat{T}, \hat{X}], \hat{H}] + [[\hat{X}, \frac{\hat{p}^2}{2m}], \hat{T}] = 0$$
$$\Rightarrow [[\hat{T}, \hat{X}], \hat{H}] + [[\hat{X}, \hat{p}]\frac{i\hbar\hat{p}}{m}, \hat{T}] = 0$$
$$\Rightarrow [[\hat{T}, \hat{X}], \hat{H}] - \frac{\hbar^2}{m}[\hat{p}, \hat{T}] = 0$$

It's not possible to postulate $[\hat{p}, \hat{T}] = 0$, because that would mean that $[\hat{H}, \hat{T}]$ is zero too. Thus in general neither $[\hat{p}, \hat{T}]$ or $[\hat{X}, \hat{T}]$ are zero and therefore no pair of these quantities can be measured simultaneously.

What does this imply for the "ideal" perception of time in Quantum Mechanics?

It implies that maybe this is the actual difficulty of the whole endeavor. We attempt to conceive a quantity expressed by a self-adjoint operator, but which quantity it's been proven, cannot be measured simultaneously to position and momentum, while the definition of the problem has right from the start specific momentum and position initial conditions and specific arrival position. Probably, this is the root of the evil [5], while others of course suggest that the problem is more fundamental [22, 6].

5.1.2 The derivation

Let's assume the commutation relation $[\hat{H}, \hat{T}] = i\hbar$ valid and the $\hat{T}$ operator self-adjoint. We can obtain the probability amplitude for this operator through $\langle\tau|\psi\rangle$. This implies the completeness relation and the orthogonality of the $|\tau\rangle$ states.

Moreover, using the completeness relation of the momentum eigenstates we can express this amplitude as a momentum integral:

$$\langle\tau|\psi\rangle = \int_{-\infty}^{\infty} \langle\tau|p\rangle\langle p|\psi\rangle \tag{5.1}$$

We can calculate the expression $\langle\tau|p\rangle$ from the commutation realation $[\hat{H}, \hat{T}] = i\hbar$. From previous chapters we know that treating properly the commutation relation we are lead to this equation:

$$\exp(-it\hat{H}/\hbar)|\tau\rangle = |\tau - t\rangle$$
$$\Rightarrow \exp(-it\hat{p}^2/2m\hbar)|\tau\rangle = |\tau - t\rangle$$

and multiplying both sides with the bra $\langle p|$:

$$\Rightarrow \langle p| \exp\left(-it\hat{p}^2/2m\hbar\right)|\tau\rangle = \langle p|\tau - t\rangle$$
$$\Rightarrow \exp\left(-itp^2/2m\hbar\right)\langle p|\tau\rangle = \langle p|\tau - t\rangle$$

Thus setting $t = \tau$:

$$\Rightarrow \exp\left(-i\tau p^2/2m\hbar\right)\langle p|\tau\rangle = \langle p|0\rangle$$
$$\Rightarrow \langle p|\tau\rangle = \langle p|0\rangle \exp\left(i\tau p^2/2m\hbar\right) \equiv A(p)\exp\left(i\tau p^2/2m\hbar\right)$$

In order to calculate $A(p)$, we use the orthogonality of the $|\tau\rangle$ states and the completeness relation of momentum:

$$\Rightarrow \int_{-\infty}^{\infty} dp\langle\tau'|p\rangle\langle p|\tau\rangle = \langle\tau'|\tau\rangle = \delta(\tau' - \tau)$$
$$\Rightarrow \int_{-\infty}^{\infty} dp|A(p)|^2 \exp\left(i(\tau' - \tau)p^2/2m\hbar\right) = \delta(\tau' - \tau)$$

By replacing $E = p^2/2m$ and $dp = m\,dE/|p|$:

$$\Rightarrow \sum_{\alpha} \int_{0}^{\infty} \frac{m\,dE}{\alpha p}|A(p)|^2 \exp\left(i(\tau' - \tau)E/\hbar\right) = \delta(\tau' - \tau)$$

Therefore, we can assign to $A(p)$ the value of:

$$A(p) \equiv \sqrt{\frac{2\pi|p|}{\hbar m}} \tag{5.2}$$

Thus we conclude for the amplitude that:

$$\langle\tau|\psi\rangle = \sqrt{\frac{2\pi}{\hbar m}} \int_{-\infty}^{\infty} dp\sqrt{|p|}\exp\left(i\tau p^2/2m\hbar\right)\langle p|\psi\rangle \tag{5.3}$$

or as a function of k:

$$\langle\tau|\psi\rangle = \sqrt{\frac{\hbar}{2\pi m}} \int_{-\infty}^{\infty} dk\sqrt{|k|}\exp\left(i\tau\hbar k^2/2m\right)\langle k|\psi\rangle \tag{5.4}$$

Finally, after a spatial translation to the position X and considering in reasonable grounds that a $|\tau\rangle$ consists only of momenta of the same sign:

$$\langle\tau|\psi\rangle_{\pm} = \sqrt{\frac{\hbar}{2\pi m}} \int_{0}^{\pm\infty} dk\sqrt{|k|}\exp\left(-ikX\right)\exp\left(i\tau\hbar k^2/2m\right)\langle k|\psi\rangle \tag{5.5}$$

We retrieve the exact same expression for the amplitude, and thus the probability distribution, with Kijowski's distribution (3.16) and with the results (4.26) and (4.81) of the two methods described in the previous chapter.

5.1.3 Commentary on the two methods

The above result doesn't render the two methods described in Chapter 4 and the Kijowski's distribution as true or consistent with what we want. We simply showed that since they were subject to the same assumptions, it was expected to end up to the same results and thus it wasn't finally so surprising. Does this mean that the previous extensive analysis was redundant? No, because the above derivation assumes the validity of the commutation relation and $[\hat{H}, \hat{T}] = i\hbar$ and the self-adjointness of the $\hat{T}$ operator. Thus, we had to argue extensively on these aspects.

And a final, commentary on the two methods. Oppenheim et al. [31] criticized the first of the methods, spotting an inconsistence on the normalization of the eigenstates of the new regulated "time" operator, which doesn't actually allow to ignore so easily the states for very small ϵ. Of course, he used a specific expression of a wave packet to justify his arguments, something which doesn't justify an assertion of generality to the arguments. Still of course, this is not a criticism to be neglected.

Indeed $k = 0$ is still a singularity point and moreover, something we don't mention explicitly before, there is a singularity point for the second method too, the $|\tau = 0\rangle$eigenstate of the $\hat{\mathcal{T}}$, since the action of the time-evolution operator on it: $e^{-i\hat{H}_0 t/\hbar}|\tau = 0\rangle$, doesn't lead univocally to a specific new state, but equivalently to $|\pm t\rangle$. For these points indeed it must be investigated exhaustingly if in the general case they lead to an inconsistency for the two aforementioned methods.

5.2 On Pauli's "Theorem" and on our "optimism"

Apart from the very interesting work of Eric Galapon on the domains of the operators considered for the commutations relation investigated by Pauli's "Theorem", we would like to commend further on it, expressing our humble perspective, always without never underestimating its significance.

The inaugural reason for the dead end on the time in Quantum Mechanics problem presented by the "Theorem", is the action of this constructed $e^{i\epsilon\hat{T}/\hbar}$ operator, ie. equation (3.14): $e^{i\epsilon\hat{T}/\hbar}|E\rangle = |E - \epsilon\rangle$. And since for non-bounded systems, negative energy states cannot be defined, we seemingly reach to an impasse.

But what is the physical meaning of the operator? Does it act like the time evolution operator: $e^{-it\hat{H}/\hbar}$? What does actually do on states? We took for granted that it "creates" new states, which are eigenstates of the $\hat{operator}$

because of the relation (3.13) we concluded: $\hat{H}\, e^{i\epsilon\hat{T}/\hbar}\, |E\rangle = (E-\epsilon)\, e^{i\epsilon\hat{T}/\hbar}\, |E\rangle$. But is this more like a transformation of coordinates rather than the creation of a new state?

We'll come back to last question, but firstly let's contemplate in general on the power series that enabled us to construct the exponential operator. For these mathematical constructions it is implied that they are defined on existing states. If we exclude states from our definition, then the power series cannot be defined either. These exponential operators won't construct new states outside of the domain in consideration. They are too confined inside it. Hence, $|E-\epsilon\rangle$ states are inside our initially domain of definition, not somewhere else scarily.

Of course, this doesn't mean that it's not a serious problem that a postulated conjugation of the Hamiltonian operator with a certain time operator is contradictory in the sense that two operators do not have the same domain of definition inside the Hilbert space. But a confined range of values for a certain parameter of the states does not render the commutation relation and the conjugation itself contradictory or impossible. The momentum-position commutation relation for example, $[\hat{x}, \hat{p}] = i\hbar$, is still valid even for a spatially confined infinite square well, for which with every momentum value is possible.

And what actually does this conjugation of Hamiltonian operator with a postulated time operator imply? The same exactly as in Classical Physics: the covariance of the conservative system in time translations. It doesn't predict the specific behavior or the limits of the system; there is not enough information for this purpose. It simply states its general behavior of covariance when a parameter changes. Thus, the commutation relation couldn't have anticipated for the range of the energy values; this have to be imposed as an additional assumption and thus still the commutation relation has much to say. The main problem is first of all the defining domains of the operators.

Moreover, due to this covariance on time transformations, we can interpret both ways the changing values of the time parameter, either as a flow of time, or as a change of the reference point in time. Is there a corresponding symmetry for time when the values of energy change? Possibly yes, but since we confine the values of energy, in contrast with the values for time, this cannot be considered that coincides well enough with the definition of symmetry. Thus this $|E-\epsilon\rangle$ energy eigenstate can be interpreted that it refers either to another state or to an arbitrary and absolutely valid change of energy levels. However in our humble opinion, this is not the main problem, merely an indication of it. And, again in our opinion, this renders the energy quantity as not always adequate to describe time, in the same way which the time parameter, via its transformation, not only describes, but defines the energy concept. We have to be careful with the latter point.

It would have been, of course, really helpful if we could manage to construct an expression for the time operator which it would cancel any states below zero, like the annihilation operator of the harmonic oscillator systems. Still, however the problem is, apart from any singularity points, the fact that we aim to the measurement of the time-of-arrival quantity using expressions of operators of position and momentum, while none of these three quantities can be measured simultaneously.

So, how do we justify our optimism? On the grounds that via a proper definition of the quantum quantity of time of arrival, which will lead to restrictions on choices of operators and the defining domain (and we mustn't be afraid of restrictions, as in Muga and Leavens' criticism), and sticking to the fact that the aim of ours is not an operator, neither a direct association with the t time parameter of the Schrödinger equation, but rather a real quantity, which will be consistent with the definition we concluded for this specific time quantity and which will admit first of all the same symmetry attribute as time in Classical Mechanics does for conserved energy, then the intuition of ours is that via all these a consistent quantity for time of arrival and a carefully defined corresponding self-adjoint operator can be incorporated validity to the arsenal of the Quantum Mechanics. Even if moreover, this operator doesn't look like much at first sight with the classical expression of the time of arrival, something researchers tend to forget, since only its average expression has to coincide with the latter in the classical limit ($\hbar \to 0$).

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