IMPERIAL COLLEGE LONDON
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MSc Quantum Fields and Fundamental Forces

The Arrival Time Problem in Quantum Mechanics, from path integrals to backflow

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Contents

Chapter 1

Introduction - The arrival time : problem and context

In this short introduction, we would like to give some details about the problem we would like to study in this dissertation. Our primary interest here is what we call here the arrival time problem. It consists in finding what is the probability that a particle crosses a specific coordinate during a time interval. At first the question may seem easy, but a closer look to the question (60 pages of closer look that you are about to read...) will reveal that it has many extraordinary counter-intuitive aspects, and some of them are just very difficult, and many questions remain unsolved today.

One of the primary aims of this work is to review the main directions that have been or still are investigated in the exploration of this question. We will particularly emphasize the fact that there seems now to exist a consistent framework of converging results through very different methods. This is particularly important, because, as we will see, one of the most important early research papers on the topic came to the conclusion that arrival time couldn't be a quantity having consistent meaning, at least from an apparatus independent point of view.

It is worh to mention the potential importance of this topic. Let us mention two areas where the investigation of the arrival time problem can have a potentially high impact: experimental particle physics, and theoretical physics. In experimental physics knowing during which interval of time a particle has the most chance to cross a coordinate (for example the coordinate that defines the position of a detector) can allow to set up optimized devices. In theoretical physics, the arrival time problem is important in the foundation of quantum mechanics, in the sense that any new information about time in general can shed some light on quantization methods can effectively be set up, for example,in extensions of traditional quantum mechanics, such as quantum field theory.

This dissertation is essentially a litterature review, and a snapshot of the current research in the area. We have divided our work in four main chapters, from chapter two to chapter five: the second chapter explores in great detail some of the major results done by early physicists. In particular, we extensively cover Allcock's work, who published a set of three of the most important papers on the topic. We also study in detail the Kijowski distribution and the contributions of the Aharonov-Bohm group. The third chapter is devoted to a very modern and elegant approach using what we call path integrals. The chapter four then uses what we call the decoherent histories approach, which is very simple mathematically speaking, and provides very insightful results, finally the fifth chapter covers what we call the backflow effect, which is the fact that under some conditions, a wave packet with positive momenta can be subject to a propagation in the negative direction (identified with an increasing probability in that negative direction).

This work is far from being exhaustive, and the amount of research papers on this topic covers much more than we we can explain in a short review like this.

Finally, before to start, it is worth to mention what would be the ideal background knowledge of the reader, particularly if he is a advanced undergraduate student or MSc student. In the explanations that have been given, it is of course assumed a good command of quantum mechanics. This includes things like solving eigenvalues equations, matching eigenstates and their derivatives and solving Schrödinger equation under a split domain, transmitted/reflected wavefunctions,etc. Mathematically speaking, some basic concept of complex analysis such as the principal part, the wick rotation, convolution/deconvolution, some basics on Laplace Transforms etc are assumed here. Familiarity with Green functions is also required. However, path integrals are not a prerequsite, as we have given an extensive explanation on how to build them.

Chapter 2

Early investigations

2.1 The Classical case

Let us consider the elementary case of a point particle of position q and momentum p, being subject to a one-dimensional motion.

We will work first the free case, which means there will be no interaction/potential term.

We know from basic mechanics that $p = mv$, and from which we immediatly have that a particle crosses the point X at the moment:

$$T = \frac{(X - q_0)m}{p_0} \tag{2.1}$$

where q_0 and p_0 are the initial position and momentum respectively. Let us notice that this equation implies that the point X is not crossed between the start of the motion and the time T, we say it is a "'first-time crossing"' of the point X, or "'first arrival times"'.

We will consider first a phase-space distribution,(an object that we find in amny areas of physics, typically in statistical physics for example) which is a function of position, momentum and time, but defined here such that

$$F(q, p \leq 0, t) = 0 \tag{2.2}$$

this means than momentum are all positive, that is, all particles move in the same positive direction (same one because we assumed the motion to be one-dimensional).

The phase-space distribution will give us the probability current

$$\Pi(T; X) = J(T; X) = \int_0^{\infty} \mathrm{d}p \, F(X, T, p) \, \frac{p}{m} \tag{2.3}$$

where the last integral can easily be rewritten using a delta function:

$$J(T;X) = \int_0^\infty \mathrm{d}p \int_{-\infty}^\infty F(q,T,p)\,\frac{p}{m}\delta(q-X) \tag{2.4}$$

it is clear from the last equation that $J(X,T)$ is a function of time only, since X is a constant in the problem studied. In fact, this equation gives us the probability distribution of first-time crossings. Hence, we have for example that the proportion of particles crossing X between T and $T+dT$ is simply:

$J(X,T)dT$

We also see from the previous equation that $J(X,T)$ can be considered as an average of the space phase function $\frac{p}{m}\delta(q-X)$, calculated with F.

Now, there are two tools we can use. First, we have the famous equation

$$x = x_0 + vt \tag{2.5}$$

which in our context, reads

$$q(q_0,p_0,t) = q_0 + p_0\frac{t}{m} \tag{2.6}$$

and that we will use together with Liouville's theorem, stating that:

$$F(q_0,p_0,0) = F(X,p=p_0,T) \tag{2.7}$$

$$\begin{aligned}\int_{-\infty}^\infty \mathrm{d}T\,\Pi(T;X)\,T &= \int_{-\infty}^\infty \mathrm{d}T\,J(T;X)T \\ &= \int_{-\infty}^\infty \mathrm{d}q_0 \int_0^\infty \mathrm{d}p_0\,F(q_0,T,p_0)\,\frac{(X-q_0)m}{p_0}\end{aligned} \tag{2.8}$$

in the last equation, we see that the factor $\frac{p}{m}$ disappears, this is because it is absorbed in the change of variable when going from the dT integral to the dq_0 integral.

We see here that there is a potential problem, since we have a denominator in p_0, while the value $p_0 = 0$ is allowed to be integrated upon. We will have therefore to assume that this pathology can be compensated by some conditions on the phase space distribution (for example, it can be a function such that $F = Q.p_0$, where Q itself has no p_0 denominator).

It has been proven that this classical result can be obained in a more mathematical way, by setting a set of axioms on Π: we choose it positive, normalized to 1 with respect to time, having some specific symetries properties to ensure a good definition of the arrival point X, and finally, we want it to have a minimum variance. All those properties are purely mathematical and lead to the same result that the one we just derived.

If the condition 2.2 does not hold, meaning, with we have a set of particles subject to a one-dimensional motion, but not going necessarily in the same direction, then we have to reformulate our previous result regarding $J(X,T)$: as formulated earlier, it does not give us the arrival time, because we can have, as a set of particle going i the $+q$ direction, another set of particles going in the $-q$ direction, and combining in such a way that the integral gives us zero, while the arrival time should obviously not be equal to zero. In this case, what we do is to separate the contribution from each sign, positive and negative, and treat them separately. We can take this into account in the integral by integrating over the absolute values of the momenta.

The positive contribution is given for positive p's:

$$J_+ = \int_0^\infty \mathrm{d}p F(X,T,p)\,\frac{p}{m} \tag{2.9}$$

while for the negative contribution, the momenta runs down from 0 to $-\infty$:

$$J_- = \int_{-\infty}^0 \mathrm{d}p F(X,T,p)\,\frac{p}{m} \tag{2.10}$$

$$split\Pi(X,t) = \int_{-\infty}^\infty \mathrm{d}p F(X,T,p)\,\frac{p}{m} = J_+ - J_- = \Pi_+ + \Pi_-$$

(2.11)

with of course

$$J = \Pi_+ - \Pi_- \tag{2.12}$$

2.2 Allcock's work

In this section, we will review the foundation work done by Allcock [1] in his famous set of articles published in 1969. Allcock basically arrived to the conclusion that it was not possible to build consistently an apparatus-independent (we also say "‘ideal"’) arrival time. If that was all, there would have been no further research, but obvioulsy things are not so simple, and the idea is that many subsequent authors arrived to results that sometimes confirmed in some aspects, sometimes contradicted, Allcock's work. Many of analytical and numerical work that have been done by these subsequent authors is based on relaxing some hypothesis, or assuming different behaviors than Allcock for some equations. It is therefore essential to have a reasonable background understanding of what Allcock did and how he obtained his result. This will help us to appreciate better the results of physicists who came after him. It is worth to mention that Allcok was not the only physicist that arrival to a negative conclusion, as Pauli, in the Encyclopaedia of Physics published in Berlin in 1958, also published a short note where he explained the impossibility of building a self-adjoint time operator, as if it was so, the spectrum of the hamiltonian wouldn't be bounded [2]. We will not talk further about Pauli's contribution; however, we will have an in-depth analysis of Allcock's work wonsidering its critical importance in the history of the subject.

He starts first with the simple case of a free wave packet, without source, nor detector, and of course no potential. Here it is assumed we have a set of states which are arrival times eigenfunctions

$$\psi_T(x,t)|\,0 \leq E \leq \infty \tag{2.13}$$

where E is simply the energy

$$E = \frac{\hbar^2 k^2}{2m} \tag{2.14}$$

That energy is positive, as we see from the boundaries of the integral. Now, because we would like to be able to use the traditional methods of measurement theory, we require states labelled by different T's to be orthogonal. But we must first set up an explicit template expression for these states:

$$\psi_T(x,t) = \frac{m^{1/4}}{\hbar^{1/2}} \int_0^\infty \frac{\mathrm{d}E}{(2\pi)^{1/2}} \frac{\psi_T(E)}{(2E)^{1/4}}\, exp[i(2mE)^{1/2}x/\hbar - iEt/\hbar] \tag{2.15}$$

Then, time covariance allows us to write:

$$\psi_T(E) = exp(iET/\hbar)\psi_0(E) \tag{2.16}$$

And then, our orthogonality condition reads:

$$< \psi_{T'}|\psi_T >= \int_0^\infty \mathrm{d}E\, exp(iEz)|\psi_0(E)|^2 \tag{2.17}$$

with $z = (T - T')/\hbar$

Now, a critical remark is that this equation 2.17 is always greater than zero when $z = 0$ (that is, when $T = T'$). Since E is ≥ 0, it is in fact possible to build an analytic continuation of this equation on z with the required boundariy values. Now, if we build up such an analytic continuation, this will mean that the scalar product in 2.17 will be zero for $T \neq T'$, which is what we want. But the problem is that this analytic continuation will necesarily imply that this scalar product will also be zero for $T = T'$, which is something we don't want! And we can't do otherwise because we know from complex analysis that the analytical continuation of a specified function with specific boundary values is unique. What we can then say, based on this contradiction, is that the concept of arrival time for a free article in a system without source nor detector , has no meaning. The next stage is then to try to relax one of those conditions to see if we can get something more interesting. Let us for example assume that there is now a source term, that we will write

$$\rho_S(x,t)\theta(x_S - x) \tag{2.18}$$

which will be confined to $x \leq x_s < leqX$, and that keeps the potential V(x) to zero when $x \geq x_s$, which is thus a region where we can still can use the free Schrödinger equation.

The wave function will then be:

$$\psi_T(x \geq x_s, t) = \frac{m^{1/4}}{\hbar^{1/2}} \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{(2\pi)^{1/2}} \frac{\psi}{(2E)^{1/4}}\, exp[i(2mE)^{1/2}x/\hbar - iEt/\hbar] \tag{2.19}$$

in this last equation, we see that the range of integration includes negative energies, but at the same time we have square- and fourth- roots of E: this justifies the need for analytical continuation. Based on this formula, we can calculate the probability for the particle to be located in the following regions, asymptotically in time:

$$lim_{t\to\infty} \int_{x_S}^{X} \mathrm{d}x|\psi(x,t)|^2 = 0 \tag{2.20}$$

for the region $[x_s, X]$, and

$$lim_{t\to\infty} \int_{X}^{\infty} \mathrm{d}x|\psi(x,t)|^2 = \int_{0}^{\infty} \mathrm{d}E\,|\psi(E)|^2 \tag{2.21}$$

for the region [X,∞]

and hence, the probability of arriving at $X \geq x_S$ asymptotically in time will be

$$P(\infty) = \int_0^\infty \mathrm{d}E\, |\psi(E)|^2 \tag{2.22}$$

with all these results, if everything is right, we should be able to set up an experiment where we could, as we would wish, use traditional measurement theory. Again we would like the orthogonality of states to be satisfied. We should then be able to decompose $\psi(E)$ over the eigenstates and write

$$\psi(E) = \int_{-\infty}^{\infty} \mathrm{d}T c(T)\psi_T(E) \tag{2.23}$$

which would then mean that

$$\begin{aligned} < \psi|\psi > &= \int_{-\infty}^{\infty} \mathrm{d}E\psi^*(E)\psi(E) \\ &= \int_{-\infty}^{\infty} \mathrm{d}T|c(T)|^2 > 0 \end{aligned} \tag{2.24}$$

but this equation is always positive, while 2.22 must be zero for any state defined exclusively with negative E's. Again we have not been able to escape contradiction, and Allcock, on the basis of this, finally comes to think that the usual language of eigenstates and scalar products (in other words, the usual quantum mechanical measurement theory) cannot help in defining a consistent arrival time definition. So, to summarize, building a "'free model without source nor detector"', didn't work, then building a "'free model without detector but with source"' didnt't work either. The obvious next stage is to see what if we add a detector in the theory. Here also, we cannot escape the contradiction of getting positive contribution from negative energies, that is , again, contradicting 2.22. So Allcock ends his work by declaring that it is not possible to define arrival time when having sources.

A key reasoning that has been made by some subsequent authors, especially Muga [3] is that the expression 2.22 for $P(\text{inf})$ is not correct. One way to see it is to realize first that for negative E's, the wave number

$$k = i\frac{2m|E|^{1/2}}{\hbar} \tag{2.25}$$

leads to evanescence and gives a contribution tied to the source. In this context, it definitely makes sense to consider a system with source. Now, the problem comes from the fact that, because $P(\text{inf})$ includes contributions from all first arrival times at x=X (over all t's), we cannot guarantee that there will be no negative energy contribution to $P(\text{inf})$. Some of the possible candidates for such contributions might indeed come from the evanescent part.

What we need to remember from all this, is that, according to Allcock, we cannot thus, at this stage, build an "'ideal"' (apparatus-independent) model for arrival time. The idea then is to see if it would be possible to build an arrival time concept that could be "'extracted"' from measurement, that is, build an aparatus-dependent model. He therefore set up a very simple θ-function type potential of the form

$$-iV_0\theta(x) \tag{2.26}$$

where $V_0 > 0$

and expressed the response in terms of an incident state $\phi_{in}(E) = \psi(E)$ (this incident state being of course defined in absence of apparatus) is given by

$$\phi_{in}(x_S \leq x \leq 0, t) = \frac{m^{1/4}}{\hbar^{1/2}} \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{(2\pi)^{1/2}} \frac{\phi_{in}(E)}{(2E)^{1/4}} exp[i(2mE)^{1/2}x/\hbar - iEt/\hbar] \tag{2.27}$$

The Schrödinger equation is obvioulsy given by

$$i\hbar\frac{\partial\phi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\phi(x,t)}{\partial x^2} - iV_0\Theta(x)\phi(x,t) \tag{2.28}$$

and we can then calculate the transmitted and reflected waves, like we do in basic quantum mechanics problems:

$$\phi_{tr}(x \geq 0, t) = \frac{m^{1/4}}{\hbar^{1/2}} \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{(2\pi)^{1/2}} \frac{\phi_{tr}(E)}{(2E)^{1/4}} exp[i(2m(E + iV_0))^{1/2}x/\hbar - iEt/\hbar] \tag{2.29}$$

$$\phi_{ref}(x_S \leq x \leq 0, t) == \frac{m^{1/4}}{\hbar^{1/2}} \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{(2\pi)^{1/2}} \frac{\phi_{ref}(E)}{(2E)^{1/4}} exp[-i(2mE)^{1/2}x/\hbar - iEt/\hbar] \tag{2.30}$$

the usual continuity conditions on these function and their derivatives help us to then deduce the energy amplitudes:

$$\phi_{tr}(E) = \frac{2}{1 + E^{-1/2}(E + iV_0)^{1/2}}\psi(E) \tag{2.31}$$

$$\phi_{ref}(E) = \frac{1 - E^{-1/2}(E + iV_0)^{1/2}}{1 + E^{-1/2}(E + iV_0)^{1/2}}\psi(E) \tag{2.32}$$

We can also calculate the absorbtion rate of the probability density, since we are using an absorbing potential:

$$-\frac{\mathrm{d}N(t)}{\mathrm{d}t} = \frac{2V_0}{\hbar}\int_0^\infty \mathrm{d}x|\phi_{tr}|^2 \tag{2.33}$$

we substitute the expression for $\phi_{tr}(x \geq 0, t)$ in this last equation and integrate, and find

$$-\frac{\mathrm{d}N(t)}{\mathrm{d}t} = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\frac{\mathrm{d}E}{(E)^{*1/4}}\int_{-\infty}^{\infty}\frac{\mathrm{d}E'}{(E')^{*1/4}}\frac{iV_0[(E'+iV_0)^{1/2}+(E+iV_0)^{*1/2}]}{E'-E+2iV_0} \\ .\,\phi^*_{tr}(E)\phi_{tr}(E')\,exp[i(E-E')t/\hbar] \tag{2.34}$$

and if we further insert here the expression for the transmitted energy amplitude, we get

$$\tilde{P}(\infty) = \int_{-\infty}^{\infty}\mathrm{d}EA(E,V_0)|\psi(E)|^2 \tag{2.35}$$

where we have defined the acceptance function $A(E, V_0)$

$$A(E,V_0) = \frac{Re[(E+iV_0)^{1/2}]}{|E|^{1/2}}\left|\frac{2E^{1/2}}{E^{1/2}+(E+iV_0)^{1/2}}\right|^2 \tag{2.36}$$

We clearly see the dependence to the apparatus in this equation, through V_0. At this stage, it is useful to define the resolution time:

$$\delta T = \frac{\hbar}{2V_0} \tag{2.37}$$

(notice that this expression is directly inspired by the time-uncertainty expression). We can then wonder in which case this dependence to the apparatus can vanish, or at least become negligible. They are indeed two potentially interesting limit cases: $V_0 \to \infty$ and $V_0 \to 0$. In the first case, the response of the apparatus becomes zero because the dominant behavior for particles is to be reflected and not absorbed. In the second case, because $V_0 \to 0$, the resolution time tends to infinity. In practice, this would mean that chances are great for the particle to be absorbed far from the point we study. As a result, in both cases, the apparatus response as we have expressed it, doesn't seem to provide an interesting way to solve our problem.

Finally, we would like to mention another result of Allcock that turned out to be very interesting. Allcok wondered if it would be possible to obtain an arrival time ditribution through the apparatus response using a deconvolution. For this, he assumed a specific relation between the arrival time amplitude $\chi(T)$ and $\psi(E)$, that same $\psi(E)$ that we used before. The assumed relation is:

$$\chi(T) = \frac{1}{\hbar^{1/2}} \int_{-\infty}^{\infty} \mathrm{d}E\, h(E)\psi(E)\, exp(-iET/\hbar) \tag{2.38}$$

he inserts the arrival time amplitude in the formula that we would expect to be statisfied for a well-designed arrival tim apparatus:

$$\int_{-\infty}^{\infty} \mathrm{d}T'\, R(V_0, T - T')\, |\chi(T')|^2 \tag{2.39}$$

where $R(V_0, T-T')$ is the apparatus resolution function. The result after integration is

$$\int_{-\infty}^{\infty} \mathrm{d}E \int_{-\infty}^{\infty} \mathrm{d}E'\, h^*(E)\, h(E')\tilde{R}(V_0, E' - E)\, \psi^*(E)\, \psi(E')e^{i(E-E')T/\hbar} \tag{2.40}$$

where $\tilde{R}(V_0, E' - E$ is the Fourier transform of $R(V_0, T - T')$

Now, the key thing to notice, is that, if E′ E » V_0, we get

$$-\frac{\mathrm{d}N(t)}{\mathrm{d}t} \approx \int_{-\infty}^{\infty} \mathrm{d}t'\, R(V_0, t - t')\, |\chi(t')|^2 \tag{2.41}$$

where

$$R(V_0, t) = 2V_0\Theta(t)\, exp(-2V_0 t) \tag{2.42}$$

In this case, the arrival time distribution is given by

$$\Pi(T) = |\chi(T)|^2 = \frac{1}{2\pi\hbar} \left| \int_0^{\infty} \mathrm{d}E\, \psi(E) exp(-iET/\hbar) \right|^2 \tag{2.43}$$

and if we then change the integration variable from E to k, we finally obtain:

$$\Pi(T) = \frac{\hbar}{2\pi m} \left| \int_0^{\infty} \mathrm{d}k\, k^2 \phi(k) exp(-i\hbar k^2 t/2m) \right|^2 \tag{2.44}$$

this expression is of fundamental importance for the rest of this issertation, because we will see that it is exactly what many other physicists obtained through totally different means, among which we can mention Kijowski [4], whose work will be studied in the next section, Grot et al. [5] or Delgado and Muga [6]. The fact that many research groups managed to find the same result through unrelated methods seems to support the existence of a conistent underlying candidate concept for arrival time.

2.3 Kijowski's arrival time distribution

Kijowski's orginal motivation was to investigate which meaning should be given to the time-energy uncertainty relations. His approach was relatively straightforward: he started from the classical case,saw what kind of "conditions/axioms" it could be deduced from, and required them for the probability density in quantum mechanics. All this correspondence has been set in the free case.

Mathematically speaking, he used a theorem he proved on positive bilinear functionals F and the conditions they must satisfy to minimize the variance

$$\int_{-\infty}^{\infty} \mathrm{d}t\, t^2\, F[\psi_t] - \left(\int_{-\infty}^{\infty} \mathrm{d}t\ \ t\, F[\psi_t]\right)^2 \tag{2.45}$$

He showed that if the functionals F of wave functions ψ over positive momenta, satisfy $\int F[\psi_t] = 1$(with ψ_t being normalized state at all time having evolved an initial state ψ_0) and $F[\bar{\psi}] = F[\psi]$, then thre exist a specific functional F_0 for which this variance will be minimum, and F_0 has the form

$$F_0[\psi] = \int \frac{\mathrm{d}p_1\, \mathrm{d}p_2}{2\pi m\hbar} \bar{\psi}(p_1)\, \sqrt{p_1\, p_2}\psi(p_2) \tag{2.46}$$

In fact, F_0 defines a class a functional, for which the averaging will be constant. The integral ranges only over positive p's since this is the condition that the theorem states regarding the wave functions. The probability for such described states will then be:

$$\Pi_+^K(t) = \Pi_+^K(t, \psi) = F_0[\psi] = \left| \int_0^{\infty} \mathrm{d}p \sqrt{\frac{p}{2\pi m\hbar}} e^{-ip^2 t/2m\hbar} \psi(p) \right| \tag{2.47}$$

where the evolved state is simply obtained by setting the hamiltonian as $p^2/2m$, since we are in a free case, and this state will thus be given by

$$\psi_t(p) = e^{-ip^2 t/2m\hbar} \psi(p) \tag{2.48}$$

if we want to include also arrivals from the right,to get the total probability dentity for arrivals at time t at the position $x = 0$, we just add another term with the range of integration that goes now from $-\infty$ to 0:

$$\Pi_+^K(t, \psi) = \left| \int_0^{\infty} \mathrm{d}p \sqrt{\frac{p}{2\pi m\hbar}} e^{-ip^2 t/2m\hbar} \psi(p) \right|^2 + \left| \int_{-\infty}^{0} \mathrm{d}p \sqrt{\frac{-p}{2\pi m\hbar}} e^{-ip^2 t/2m\hbar} \psi(p) \right|^2 \tag{2.49}$$

This result is beautiful because it matches what we have found at the end of our previous section about Allcock's work, and we see that indeed the results agree with each other, because the equation is exactly the same than Allcock's. However a new problem is raised: even though this probability density seems to be consistent and to make sense, the arrival time operator will not be self-adjoint, nor even having a self-adjoint extension. And we know from all our basic quantum mechanics that self-adjoint operators are essential objects that help us in finding observed results, since eigenvalues of self-adjoint operators are real. On another hand, a more deep reason why operators should usually be self-adjoint comes from the probabilistic nature of qantum mechanics, and more exactly from the spectral theorem, which says that when we measure an observable, if the operator that describes it is self-adjoint, then the moments of probability distribution will be given by the moments of the operator. What we will do in the subsequent sections is to work in this more sophisticated probabilistic mindset and try to find a solution to our problem through the exploration of a new concept: the concept of positive operator valued measure, or, in short, POVM.

2.4 Positive operator valued measures

Let σ be the subset of a bigger set giving all the possible values of an observable. Let us call p_σ the probability associated to it. That probability is linear with respect to the density operator $\hat{\rho}$, so we must have an operator $\hat{A}_\sigma$ such that

$$p_\sigma = Tr(\hat{A}_\sigma \hat{\rho}) \tag{2.50}$$

Now, the idea is that we want those probabilities to be additive for sets of σ's that do not cross, but at the same time, if they cross, we don't want the probabilities to be counted twice. This means we want:

$$\begin{gathered} \hat{A}_{\sigma\cup\sigma'} = \hat{A}_\sigma + \hat{A}'_\sigma \ \Leftrightarrow \sigma \cap \sigma' = 0 \\ \hat{A}_{\sigma\cup\sigma'} = \hat{A}_\sigma \ \Leftrightarrow \sigma' \subset \sigma \end{gathered} \tag{2.51}$$

this will allow us to sum all the probabilities to 1:

$$1 = \sum_\sigma p_\sigma = Tr\left(\sum_\sigma \hat{A}_\sigma \hat{\rho}\right) \tag{2.52}$$

and since this is valid for all $\hat{\rho}$, we can write:

$$\hat{1} = \sum_{\sigma} \hat{A}_{\sigma} \tag{2.53}$$

The key remark now is that all the probabilities being positive, $\hat{A}_{\sigma}$ must be a positive operator. That is, our observable maps subsets σ's to to the space of positive operators, with the the conditions we just stated on additivity and summing to unity being satisfied. We say that the observable is associated to a "'positive operator valued measure"' [7].

We have said in the previous section that the purpose of introducing POVM's was to help getting more insight on the pathology of no-self ajointness of potentially interesting operators candidates. A good intermediate step is to see if it can help with some more elementary operators, and then only, once we will have gained more confidence with a simple case, study properly what POVM's bring us in our understanding of the arrival time problem. As an example then, let us have a look to the momentum operator $\hat{p} = -i\hbar\partial_x$, defined on $H_> = L^2(R^+, dx) \equiv D(\hat{p})$ [8]. The set of eigenfunction we can define from this, typically forms a complete basis:

$$\int_{-\infty}^{\infty} \mathrm{d}p \bar{\psi}_p(x')\psi_p(x) = \delta(x - x') \tag{2.54}$$

but we do not have orthogonality due to the existence of a principal part in the scalar product:

$$\int_{0}^{\infty} \mathrm{d}x \bar{\psi}_{p'}(x)\psi_p(x) = \frac{1}{2}\delta(p - p') + \frac{i}{2\pi} P \frac{i}{p - p'} \tag{2.55}$$

Now, if we consider the operator $\hat{x}$, defined on functions that are square integrable on the half line, we have that indeed it will be self-adjoint. But we have $[\hat{x}, \hat{p}] = i\hbar$ on any dense domain. Because the x operator is bounded from below, we can use Pauli's theorem we mentioned briefly previously in this work, to deduce that indeed the momentum operator defined on the half-line is not self-adjoint and admits no self-adjoint extension on $H_>$. So here we have a simpler case of our previous problem, let us see how POVM's can help.

In this case, the POVM maps intervals of the real line (because our domain is the half-line) to positive operators that satify the properties we have stated from them. The map is simply, for ϕ, $\psi \in H_>$:

$$< \phi|F([a,b])\psi >= \int_a^b \mathrm{d}p \int_0^\infty \mathrm{d}x \int_0^\infty \mathrm{d}y \bar{\psi}(x)\psi_p(x)\bar{\psi}_p(y)\psi(y) \tag{2.56}$$

we can reconstruct the action of the operator

$$(\hat{p}\phi)(x) = \int_{-\infty}^\infty \mathrm{d}p \int_0^\infty \mathrm{d}y\, p\psi(x)\bar{\psi}_p(y)\phi(y) \tag{2.57}$$

and this will give us the probability distribution associated to a state ϕ

$$\Pi_\phi(p) = \left| \int_0^\infty \mathrm{d}x\, \bar{\psi}_p(x)\,\phi(x)\right|^2 \tag{2.58}$$

one way to better see the connection between POVM and the probability distribution is to write the expectation value on a specific state ϕ as intermediate step:

$$\begin{aligned} < \phi|F(dp)\phi > &= \int_0^\infty \mathrm{d}x \int_0^\infty \mathrm{d}y \bar{\phi}(x)\frac{e^{ip(x-y)/\hbar}}{2\pi\hbar}\phi(y)\,dp \\ &= \Pi_\phi(p)\,dp \end{aligned} \tag{2.59}$$

where we have symbolically written F(dp)

finally, it is worth to mention an important property of POVM's which is covariance under displacements:

$$< \phi|e^{iq\hat{x}/\hbar}F([a,b])e^{-iq\hat{x}/\hbar}\psi >=< \phi|F([a+q,b+q])\psi > \tag{2.60}$$

this can be written more simply in terms of probability density

$$\Pi_{\psi_q}(p) = \Pi_\psi(p+q) \tag{2.61}$$

here $\psi_q = e^{-iq\hat{x}/\hbar}\psi$ is the shifted state

so far, that was for pure state. in the case of mixed states, the generalization is quite easy and will only require to now use the density operator. In position reprsentation, we will have:

$$\Pi_\rho(p) = \int_0^\infty \mathrm{d}x \int_0^\infty \mathrm{d}y \frac{e^{ip(x-y)/\hbar}}{2\pi\hbar}\rho(x,y) \tag{2.62}$$

The next stage in our reasoning is to make use of a very powerfyl theorem called Naimark's Dilation Theorem. It is a unicity theorem. In essence, it says that is we manage to build a POVM's over a certain domain, and that we extend that domain, and then try to build a new POVM on that new domain, this newly built POVM's will have exactly the same form than the initial one when restricted to the old domain (up to isomorphisms). Mathematically speaking, we assume that the operator $\hat{A}$ over a certain Hilbert space, and under the condition that this operator is maximally symmetric over the domain, there will be a unique POVM F_A such that the first operator moment coincides with the operator.The important point here to notice is that the number of extensions are potentially infinite, but not the POVM.

Now, the momentum operator defined on the half-line is indeed maximally symmetric. The natural extension we can think of is the entire real line

$$L^2(\mathbf{R}, dx) = L^2(\mathbf{R}^+, dx) \oplus L^2(\mathbf{R}^-, dx) \tag{2.63}$$

and over the full line, the momentum operator will be self-adjoint, so we can use spectral theory we are familiar with, and we will have of course for the projection valued measure E

$$< \phi|E([a,b])\psi >= \int_a^b \mathrm{d}p \int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}y \bar{\psi}(x)\psi_p(x)\bar{\psi}_p(y)\psi(y) \tag{2.64}$$

to summarize, we have set up the following recipe :

1) check that the operator is maximally symmetric, to make sure we are satisfying the conditions of the theorem 2) we then consider an extension through a certain ismorphism 3) we get the probability density on that extension , using usual spectral theory 4) the restricted probability density will give then the right POVM, guaranteed by the unicity stated by Naimark's Theorem 5) being a POVM in nature, it contains in essence the information regarding the actual experiment results (cf. the σ we used above and how they were associated to probabilities)

2.5 A short note on the concept of deficiency

We can have more insight on the self-adjointness of an operator by using the concept of "'deficiency"'[8]. Let us denote N(b) the space of eigenvectors of eigenvalue b. We will illustrate the concept of deficency by studying the operator adjoint to $\hat{p}$ defined over the half-line. Its domain must be $D(\hat{p}) \oplus N(i) \oplus N(-i)$. From this information we can construct a set of two numbers (dim(N(i)), dim(N(-i))), where dim(...) simply means the dimension of the mentioned space. Those dimensions are called deficiency indices. In the case of the operator $\hat{p}$, it gives (1,0). A self-adjoint operator would have had deficiency indices of (0,0), as well as "'essentially self adjoint"' operator, that is, those which are not self adjoint but that can be uniquely extended into self-adjoint ones. The analysis of deficiencies is a simple way to check the self-adjointness. In this case, since one of the indices is zero, while both are different, and that $\hat{p}$ is symmetric over its domain, we say that it is a maximally symmetric operator, and from what we have seen before, it has no self adjoint extension over its domain.

$$D(\hat{p}) \oplus N(i) \oplus N(-i) \tag{2.65}$$

2.6 Aharonov-Bohm operator

Aharonov and Bohm [9] investigated the construction of time operators in a study of time-energy uncertainty relations. The basic inspiration is a symmetrization of the classical expression for time t=mx/p. The arrival time at x=0 will classically be t = -mx/p, and this will naturally give us the symmetrized operator:

$$\hat{T}_{AB} = -\frac{m}{2}(\hat{x}\hat{p}^{-1} + \hat{p}^{-1}\hat{x}) \tag{2.66}$$

it is worth to have a close look at the commutation relation of this Aharonov-Bohm operator with the free operator, and we find:

$$[\hat{H}_0, \hat{T}_{AB}] = i\hbar \tag{2.67}$$

using this with the Heisenberg equation of motion, this will give the temporal dependency of de Aharonov-bohm operator, we straightforwardly get $d\hat{T}/dt = -1$

to understand what it actually means, we can imagine this simple situation: if we have a particle moving in space, at some time t, the arrival time associated to it will have a certain value T, but then, later (that is, at t'>t), the arrival time associated to this new position will be shorter since it the particle gets closer to the target-position we are interested in. From this perspective, the arrival time must naturally flow at an opposite rate with respect to teh usual parametric time, and this is exactly the meaning of $d\hat{T}/dt = -1$.

Now, one thing to notice is that this operator, again, is not self-adjoint. We will therefore use the tools we have previoulsy developped to cure this pathology. The first aspect we have to have a look at is the domain of this time operator. Is is more convenient to study it in momentum representation

$$\hat{T}_{AB} \rightarrow \frac{i\hbar m}{2}\left(\frac{1}{p^2} - \frac{2}{p}\frac{\partial}{\partial p}\right) \tag{2.68}$$

there is a clear singularity at p=0, so we will need wavefunctions that makes this singularity irrelevant. We can show that suitable ψ's are those such that

$$p \rightarrow 0 \;\Leftrightarrow\; \psi(p)/p^{3/2} \rightarrow 0 \tag{2.69}$$

and we require also the symmetry of the time operator, which is the case as it is in fact maximally symmetric.

Now, we would like to have a look at the deficiencies. For this, we first study the expression

$$< \psi|\left(\hat{T}_{AB} + i\right)\phi >= 0 \tag{2.70}$$

which is satisfied if $\psi isaneigenvectorof^{+}_{AB}$ of eigenvalue i.We find two eigenvectors:

$$\psi_{\pm}(p) = \Theta(\pm p)\,\sqrt{\pm p}e^{-p^2/2m\hbar} \tag{2.71}$$

We then do the same with the eigenvalue -i and it appears that there are none. Therefore, the deficiencies are (2,0) and we see that no self-adjoint extension exists. We will then have to do the same analysis that what we did previously for the momentum defined on the half line. To make our study simpler, we will first switch to the energy representation. This will also make easier to compare with some of the previous results, as for example, we remember that Allcock wrote some of his results in energy representation.

We first decompose the Hilbert space H_p in two subspaces that will be associated in positive and negative momenta:

$$\begin{aligned} L^2(\mathbf{R}, dp) &= L^2(\mathbf{R}^+, dE) \oplus L^2(\mathbf{R}^-, dE) \\ &= H_+ + H_- \end{aligned} \tag{2.72}$$

the correspondence between the momentum and energy description is given by:

$$\begin{aligned} \psi_{\pm}(E) &= \left(\frac{m}{2E}\right)^{1/4} \psi(\pm\sqrt{2mE}) \\ \psi(p) &= \left(\frac{|p|}{m}\right)^{1/2}\left[\Theta(p)\psi_{+}\left(\frac{p^2}{2m}\right) + \Theta(-p)\psi_{-}\left(\frac{p^2}{2m}\right)\right] \end{aligned} \tag{2.73}$$

in fact, it appears that under this isomorphism, the switch to energy representation makes the time operator to become simply $-i\hbar\partial_E$, leading to the isomorphism:

$$\begin{aligned}\hat{T}_{AB} &= (-i\hbar\partial_E) \oplus (-i\hbar\partial_E) \\ &= \hat{T}_+ \oplus \hat{T}_-\end{aligned} \tag{2.74}$$

we should bear in mind that in energy representation, we have degenerate states:

$$\begin{aligned}\psi_+^{(t)}(E) &= \left(\frac{1}{\sqrt{2\pi\hbar}}e^{iEt/\hbar}, 0\right) \\ \psi_-^{(t)}(E) &= \left(0, \frac{1}{\sqrt{2\pi\hbar}}e^{iEt/\hbar}\right)\end{aligned} \tag{2.75}$$

which give through the isomorphism the form

$$\tilde{\psi}_\alpha^{(t)}(p) = \Theta(\alpha p)\left(\frac{\alpha p}{2\pi m\hbar}\right)^{1/2} e^{ip^2t/2m\hbar} \tag{2.76}$$

a good idea is to use Dirac's notation

$$< p|t, \alpha >= \tilde{\psi}_\alpha^{(t)}(p) \tag{2.77}$$

we have obviously

$$\sum_\alpha \int_{-\infty}^{\infty} \mathrm{d}t|t, \alpha >< t, \alpha| = 1 \tag{2.78}$$

but the states are not orthogonal due to the exisence of a principal part, a problem we are now familiar with:

$$\begin{aligned}< t', \alpha'|t, \alpha > &= \int_0^\infty \mathrm{d}E\psi_{\alpha'}^{(t')}(E)\psi_\alpha^{(t)}(E) \\ &= \int_{-\infty}^{\infty} \mathrm{d}p\tilde{\psi}_{\alpha'}^{(t')}(p)\,\tilde{\psi}_\alpha^{(t)}(p) \\ &= \frac{1}{2}\delta_{\alpha\alpha'}\left(\delta(t-t') + \frac{i}{\pi}P\frac{1}{t-t'}\right)\end{aligned} \tag{2.79}$$

the natural step at this stage is to calculate the POVM for the measures of the Aharonov-Bohm time operator. In energy representation, it is:

$$\Pi^K_{(\psi_+,\psi_-)}(t) = \left|\int_0^\infty \mathrm{d}E\frac{e^{-iEt/\hbar}}{\sqrt{2\pi\hbar}}\psi_+(E)\right|^2 + \left|\int_0^\infty \mathrm{d}E\frac{e^{-iEt/\hbar}}{\sqrt{2\pi\hbar}}\psi_-(E)\right|^2 \tag{2.80}$$

while in momentum representation it reads

$$\Pi^K_{(\psi)}(t) = \left| \int_0^\infty \mathrm{d}p \left(\frac{p}{2\pi m\hbar}\right)^{1/2} e^{-ip^2t/2m\hbar}\psi(p) \right|^2 + \left| \int_{-\infty}^0 \mathrm{d}p \left(\frac{-p}{2\pi m\hbar}\right)^{1/2} e^{-ip^2t/2m\hbar}\psi(p) \right|^2 \quad (2.81)$$

which we can write more simply:

$$\Pi^K_{(\psi)}(t) = | < t, +|\psi > |^2 + | < t, -|\psi > |^2 \quad (2.82)$$

again, we have found the now familiar Kijowski distribution. We see thus that the Aharonov-Bohm time operator in the free case agrees with Kijowski distribution, itself completey agreeing with the last result we mentioned in our section regarding Allcock's work.

Chapter 3

The path integral approach

3.1 The concept of path integral

Path integrals are a very powerful tool that is used in todays research as an alternative method to the canonical quantization in quantum field theory. It is mathematicaly less heavy, and physically more meaningful. It also provides an elegant mindset that gives answers to some philosophical questions which arised at the time of the Enlightement, especially regarding the reason for the existence of least action principles. An extensive coverage of this concept can be found in a now classical book written by Feynman and Hibbs. Here we will give an outline of what it is, and how it can be expressed mathematically. We will later use a tool called "'path integral expansion"' that will be one of our first-hand tool in our investigations on the arrival time problem.

Let us first make clear what we mean by the word "'path"'. One of the approaches is based on a heuristic generalization of the well-known double slit experiment. In that famous experiment, we have a source A, and, say, a detector B, separated by a screen that contains two slits A_1 and A_2. Particles are emitted from the source, and are supposed to arrive at the detector after having gone through the slits. Now, this experiment can be generalized in two ways:

(i) first, we can increase the number of screens between the source and the detector indexed, say, with a letter j screens
(ii) second, we can also decide to put more than two slits in a screen, and put, a number of them indexed by a letter n

As a result, the history of a detected particle will be both a function of j and n, a particular $A_{j,n}$ (nth slit of the screen A_j. To go from the source A to the detector B, the particle will have to go through a sequence of such $A_{j,n}$. Now the idea is to take a double limit where both the number of slits,and number of screens, go to infinite. Then, the limit of the sequence $A_{j,n}$ is a "'path"'.

What we will need in this work is a path integral expression for the fundamental quantity we need, that is, the amplitude from x_a to x_b in a duration of T:

$$U(x_a, x_b, T) = < x_b|\hat{U}(T)|x_a > \tag{3.1}$$

with of course

$$\hat{U}(T) = e^{-iT\hat{H}/\hbar} \tag{3.2}$$

and $\hat{H}$ being the usual non-relativistic hamiltonian.

Now the idea is to set

$$T = \epsilon.N \tag{3.3}$$

we have thus N short intervals of duration ϵ. This will give us:

$$\hat{U}(T) = \hat{U}(\epsilon)^N \tag{3.4}$$

we can then rewrite the evolution operator in terms of N different products:

$$U(x_a, x_b, T) = < x_b|\hat{U}(\epsilon)\hat{U}(\epsilon)...\hat{U}(\epsilon)|x_a > \tag{3.5}$$

But because we have the completeness

$$1 = \int \mathrm{d}x_k \; |x_k >< x_k| \tag{3.6}$$

we have

$$U(x_a, x_b, T) = \int \mathrm{d}x_1...\mathrm{d}x_{N-1} \prod < x_{k+1}|\hat{U}(\epsilon)|x_k > \tag{3.7}$$

here the product runs from $k = 0$ to $k = N - 1$.

Because the intervals are small enough, we can approximate the evolution operator by its first order Taylor expansion:

$$< x_{k+1}|\hat{U}(\epsilon)|x_k > \approx < x_{k+1}|(1 - i\epsilon\hat{H}/\hbar)|x_k > \tag{3.8}$$

Let us remember that the hamiltonian is typically a function of not only the coordinates but also the conjugate momentum, so a good idea at this stage is to insert a set of momentum states, which we can do since they are also subject to completeness. The Hamilton term of the above expression can thus be written:

$$\begin{aligned} < x_{k+1}|\hat{H}|x_k > &= \int \mathrm{d}p_k < x_{k+1}|\hat{H}|p_k >< p_k|x_k > \\ &= \int \mathrm{d}p_k\, H\; < x_{k+1}|p_k >< p_k|x_k > \end{aligned} \tag{3.9}$$

here we can use

$$< p_k|x_k >= \frac{1}{\sqrt{2\pi\hbar}} exp(-ipx/\hbar) \tag{3.10}$$

which leads to

$$< x_{k+1}|\hat{H}|x_k >= \int \frac{\mathrm{d}p_k}{2\pi\hbar}\, H\, e^{\frac{i}{\hbar}p_k(x_{k+1}-x_k)} \tag{3.11}$$

This last equation gives us the infinitesimal evolution operator:

$$< x_{k+1}|\hat{U}(\epsilon)|x_k >= \int \frac{\mathrm{d}p_k}{2\pi\hbar} e^{\frac{i}{\hbar}p_k(x_{k+1}-x_k)-\epsilon H} \tag{3.12}$$

this will finally give us the "'macroscopical"' amplitude $U(x_a, x_b, T)$:

$$U(x_a, x_b, T) = \int \prod_{j=1}^{N-1} \mathrm{d}x_j \prod_{k=0}^{N-1} \frac{\mathrm{d}p_k}{2\pi\hbar} \{\, e^{\frac{i}{\hbar}p_k(x_{k+1}-x_k)-\epsilon H}\, \} \tag{3.13}$$

the x and p integrals are often writen $\int \mathcal{D}x\mathcal{D}p$. We can write the argument of the exponential in a more meaningful way by noticing that $x_{k+1} - x_k$ can be replaced by $\epsilon\dot{x}$. This will make appear a dt integral:

$$U(x_a, x_b, T) = \int \mathcal{D}x\mathcal{D}p\{\, e^{\int_0^T \mathrm{d}t\, \frac{i}{\hbar}p\dot{x}-H}\, \} \tag{3.14}$$

This integral can be calculated explicitly in the case of a non-relativistic hamiltonian, which is just the familiar total energy:

$$H = \frac{p^2}{2m} + V \tag{3.15}$$

and we finally obtain, after some algebra:

$$U(q_a, q_b, T) = \int_{q(0)=q_a}^{q(T)=q_b} \mathcal{D}q(t) exp\{\frac{i}{\hbar}\int_0^T \mathrm{d}t L(q, \dot{q})\} \qquad (3.16)$$

This formula gives what we call a "'path integral"' giving the amplitude from q_a to q_b. Notice that we have replaced our x's by the generalized coordinated q'z, but there will not be any confusion here about this. This path integral can easily be extended to the many-particles case. The key thing to notice, is that the integrand here is nothing else than the action S! This integrand have a huge oscillation behavior when the action is non negligible, but most of the contributions will actually cancel the integral except those for which the variation of the action with respect to q is zero. This is exactly the least action principle that we knew from classical mechanics. From this perspective, the least action principle and its corollaries (like Maupertuis principle) can be seen as a consequence of the relevance of the concept of path integrals.

3.2 Introduction to path decomposition expansions

The path decomposition expansion (simply called PDX), in essence, is a method that is based on the partitioning of the configuration space in several regions, for which we individually define a suitable Green function [10], that we calculate using an adequate approximation. Because of this splitting into different regions, each one having its own description, we easily understand why this method is quite powerful.

Because it is based directly in Green functions, it is good to have a first look into PDX's in terms of Green functions, to see how these two mathematical concepts relate to each other. After that, we will give a path integral derivation for what we will call from now the "'PDX formula"'. The derivation of that formula will be the main objective of this section, as this is the very tool we will use later in this dissertation in analysing path integral methods in the arrival time problem.

Because we would like to explore a situation where the configuration space is divided into two regions, we can consider the typical case of an electromagnetic field. The Hamiltonian will be given by:

$$H = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \frac{e}{c}A(x)\right)^2 + V(x) \qquad (3.17)$$

As we know, the Green's function will be defined as follows:

$$(H(x) - E)G(x, y, E) = (H(y)^* - E)G(x, y, E) = \hbar\delta(x - y) \tag{3.18}$$

or, in operator form:

$$G(E) = \frac{1}{H - E - i\epsilon} \tag{3.19}$$

We will denote Σ the surface that separates the two regions we will study. We can obviously make a distinction in two classes of points: those which are inside Σ, and those which are outside.

If x and y are outside of Σ, and writing:

$$\begin{aligned} &G^{(r)}(y, z, E)\left((H(z) - E)G(z, x, E) - \hbar\delta(z - x)\right) \\ &\quad = \left((H(z)^* - E)G^{(r)}(y, z, E) - \hbar\delta(y - z)\right)G(z, x, E) \end{aligned} \tag{3.20}$$

we can z-integrate outside Σ and obtain:

$$G(y, x, E) = G^{(r)}(y, x, E) + \int_\Sigma \mathrm{d}_\Sigma z G^{(r)}(y, z, E)[\Sigma(z)]G(z, x, E) \tag{3.21}$$

where we have used the condensed notations:

$$\begin{aligned} [\Sigma(z)] &= \frac{i}{2}n(z).(\overrightarrow{p(z)} - \overleftarrow{p(z)^*}) \\ p(z) &= \frac{1}{m}\left(\frac{\hbar}{i}\frac{\partial}{\partial z} - \frac{e}{c}A(z)\right) \end{aligned} \tag{3.22}$$

Here n(z) is just the vector perpendiculat to the surface and pointing outward, defining its orientation.

Now, the thing to notice, is that the first term of the right-member in 3.21 is zero if x in inside the surface and y is outside:

$$G(y, x, E) = \int_\Sigma \mathrm{d}_\Sigma z G^{(r)}(y, z, E)[\Sigma(z)]G(z, x, E) \tag{3.23}$$

that last formula is the generic form of a path integral expansion. It can be generalized to any type of partitioning of the configuration space.

We will now derive that formula in another way, using path integrals. We will actually find the same formula that the generic one above, but in a simpler form that will be more suitable to our needs in this dissertation. We know that the evolution kernel K(y,x,t) satisfies

$$\begin{aligned} (H - i\hbar\partial_t)K = 0 \\ lim_{t\to 0}K(y,x,t) = \delta(y-x) \end{aligned} \tag{3.24}$$

and this kernel relates to the Green's function through a Laplace transform:

$$G(y,x,E) = i\int_0^\infty \mathrm{d}tK(y,x,t)e^{iE(t+i\epsilon)/\hbar} \tag{3.25}$$

which means that we can write Green's functions in terms of kernels. For example, if we consider again the case where x is inside the surface and y is outside, we get:

$$K(y,x,T) = i\int_0^T \mathrm{d}t\int_\Sigma \mathrm{d}_\Sigma z K^{(r)}(y,z,t)[\Sigma]K(z,x,T-t) \tag{3.26}$$

which is obviously again a PDX-type formula. Here, $K^{(r)}$ is, like $G^{(r)}$, a restriction of K. This equation can be interpreted in terms of probability of going from x to y, splitting it into the probability of going from x to z, and from z to y, without crossing te surface once it has been crossed once (hence the meaning of the restriction).

Now, working in terms of kernel or working in terms of evolution operators being equivalent, we can use the path integral formalism, since, as we have seen in the previous section, its foundation object is indeed the evolution operator. We use in fact:

$$K(y,x,T) = \int_{x(0)=x}^{x(T)=y} \mathcal{D}x(t)\ exp[iS(x(t))/\hbar] \tag{3.27}$$

Similarly to what we have seen for $G^{(r)}$ before, $K^{(r)}$ will give zero at the surface, so that the path integral for $K^{(r)}$ will only deals with paths that don't cross the surface.

Now, we can have more insight on the probability aspect by doing a Wick rotation on time in the equation for K. We apply the transformation $t \to -it$. This procedure is quite standard in physics. It is used, for example, in showing striking correspondences between statistical mechanics and some areas of quantum field theory, like the existence of critical exponents or other thermodynamics-type properties, by switching into euclidean quantities. Here, we obtain an euclidean kernel and action:

$$\begin{aligned} K_{eucl}(y,x,T) &\equiv K(y,x,-iT) \\ &= \int_{x(0)=x}^{x(T)=y} \mathcal{D}x(t)\ exp[-S_{euclidian}(x(t))/\hbar] \end{aligned} \tag{3.28}$$

and the PDX equation we had for K becomes

$$K_{eucl}(y,x,T) = -\int_0^T \mathrm{d}t \int_\Sigma \mathrm{d}_\Sigma z\, K_{eucl}^{(r)}(y,x,t)[\Sigma]K(z,x,T-t) \tag{3.29}$$

it is this last equation that will be of interest to us. Let us consider first a discrete one-dimensional situation:

$$\begin{aligned} K_N(y,x,T) &= \left(\frac{m}{2\pi\hbar\epsilon}\right)^{N/2} \int_{-\infty}^{\infty} \prod_{i=1}^{N-1} dx_i\, exp(-\frac{1}{\hbar}\sum_{j=0}^{N-1} U_\epsilon(x_j,x_{j+1})) \\ U_\epsilon(x_j,x_{j+1}) &= \frac{m}{2\epsilon}(x_{j+1}-x_j)^2 + \epsilon V(x_j) \end{aligned} \tag{3.30}$$

we must have of course that $K_N(y,x,T) = lim_{N\to\infty} K_{eucl}(y,x,T)$. Denoting $x_0 = x$, $x_N = y$ and $T = \epsilon N$ (a trick we already used in the previous section , when we introduced the concept of path integration), we notice that for each interval $[i\epsilon,(i+1)\epsilon]$, there is the possibility of a last crossing. This allows us to write then:

$$\begin{aligned} K_N(y,x,T) = \sum_{i=0}^{N-1} &\left(\frac{m}{2\pi\hbar\epsilon}\right)^{N/2} \int_{-\infty}^{\infty} \prod_{j=1}^{i-1} \mathrm{d}x_j exp(-\frac{1}{\hbar}\sum_{j=0}^{i-1} U_\epsilon(x_j,x_{j+1})) \\ &\cdot \int_{-\infty}^{z} \mathrm{d}x_i exp(-\frac{1}{\hbar}U_\epsilon(x_i,x_{i+1})) \\ &\cdot \int_z^{\infty} \prod_{j=i+1}^{N-1} \mathrm{d}x_j exp(-\frac{1}{\hbar}\sum_{j=i+1}^{N-1} U_\epsilon(x_j,x_{j+1})) \end{aligned} \tag{3.31}$$

will now use an identity without proof [11]:

$$\begin{aligned} \sqrt{\frac{m}{2\pi\hbar\epsilon}} exp(-\frac{m(x_{i+1}-x_i)^2}{2\hbar\epsilon}) = &\int_0^\epsilon \mathrm{d}\tau \sqrt{\frac{m}{2\pi\hbar\tau}} exp(-\frac{m(z-x_i)^2}{2\hbar\tau}) \\ &\cdot \frac{\hbar}{m}\frac{\partial}{\partial z}\left(\sqrt{\frac{m}{2\pi\hbar(\epsilon-\tau)}} exp(-\frac{m(x_{i+1}-z)^2}{2\hbar(\epsilon-\tau)})\right) \end{aligned} \tag{3.32}$$

and we obtain

$$K_N(y,x,T) = \sum_{i=0}^{N-1} \int_0^{\epsilon} \mathrm{d}\tau \left(\frac{m}{2\pi\hbar\epsilon}\right)^{i/2} \sqrt{\frac{m}{2\pi\hbar\tau}} \int_{-\infty}^{\infty} \prod_{j=1}^{i-1} \mathrm{d}x_j \int_{-\infty}^{z} \mathrm{d}x_i$$
$$.exp(-\frac{1}{\hbar}[U_\tau(x_i,z) + \sum_{j=0}^{i-1} U_\epsilon(x_j,x_{j+1})])\frac{\hbar}{m}\frac{\partial}{\partial z}(R(\frac{m}{2\pi\hbar\epsilon})^{N-i-1/2}\sqrt{\frac{m}{2\pi\hbar(\epsilon-\tau)}} \tag{3.33}$$
$$.\int_z^{\infty} \prod_{j=i+1}^{N-1} \mathrm{d}x_j exp(-\frac{1}{\hbar}[U_{\epsilon-\tau}(z,x_{i+1}) + \sum_{j=i+1}^{N-1} U_\epsilon(x_j,x_{j+1})]))$$

where we have set $R = exp(-(\epsilon-\tau)[V(x_i) - V(z)]/\hbar$. When we take the continuous limit, R will be equal to one, that is, not contributing as a factor. Also, we have

$$\int_z^{\infty} \mathrm{d}x_i exp(-U_\tau(x_i,z)/\hbar) = \int_{-\infty}^{z} \mathrm{d}x_i exp(-U_\tau(x_i,z)/\hbar)\hat{R} \tag{3.34}$$

where we have set $\hat{R} = exp(-\tau[V(2z-x_i) - v(x_i)]/\hbar$, which will also give 1 at the continuous limit. As a result of all this, $\int_z^{\infty} dx_i$ can be rewritten $(1/2)\int_{-\infty}^{\infty} dx_i$, and we get

$$K_N(y,x,T) = \int_0^T \mathrm{d}t K_{N1}(z,x,t)\frac{\hbar}{2m}\frac{\partial}{\partial z}K_{N2}^{(r)}(y,z,T-t) \tag{3.35}$$

with is what we were looking for. It is this formula that we will now use, but with propagators.

3.3 path decompositions and complex potentials

What we will do now is to use the path integral techniques we have developped to calculate propagators of the type

$$g(x_1,\tau|x_0,0) =< x_1|exp(-iH_0\tau - V_0\theta(-\hat{x})f(\hat{x})\tau|x_0 > \tag{3.36}$$

where x_1 can be positive and negative, but x_0 will always be chosen positive.

From what we have seen in previous sections, we can write:

$$g(x_1,\tau|x_0,0) = \int \mathcal{D}x\, exp(iS) \tag{3.37}$$

with

$$S = \int_0^\tau \mathrm{d}t \left(\frac{1}{2} m\dot{x}^2 + iV_0\theta(-x)f(x) \right) \tag{3.38}$$

Now, because there is a θ-function, we will need to split between x<0 and x>0. For this we will use the PDX methods [13].

Let us first imagine that we have $x_1 \leq 0$ and $x_0 \geq 0$. Since a path that crosses x=0 must have a first crossing, this means that, between the initial time and the first crossing, the portion of that path is all contained in the positive x's, and we can therefore write

$$g(x_1, \tau|x_0, 0) = \frac{i}{2m} \int_0^\tau \mathrm{d}t_1\, g(x_1, \tau|0, t_1)\, \frac{\partial g_r}{\partial x}(x, t_1|x_0, 0)|_{x=0} \tag{3.39}$$

Similarly, if we would like now to write an expression involving the last crossing, then it means we are talking about a portion of path that is entirely restricted between x=0 and x_1. The restriction guarantees that the path does actually not change sign, meaning, it stays in the required interval, hence the fact that the corresponding crossing at x=0 is a "'last crossing"'. We can thus write:

$$g(x_1, \tau|x_0, 0) = -\frac{i}{2m} \int_0^\tau \mathrm{d}t_2\, \frac{\partial g_r}{\partial x}(x_1, \tau|x, t_2)|_{x=0}\, g(0, t_2|x_0, 0) \tag{3.40}$$

We can even write a more exotic expression, involving a first and last crossing: there will be a restriction between the initial point and x=0, a restriction of the path between x=0 and the final point, and, also, a propagator that will carry the information that relates to what happened between the first and last crossing of x=0, and which mathematically takes the form of a propagator "'between zero and zero"', so to say:

$$g(x_1, \tau|x_0, 0) = \frac{1}{4m^2} \int_0^\tau \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1\, \frac{\partial g_r}{\partial x}(x_1, \tau|x, t_2)|_{x=0}\, g(0, t_2|0, t_1)\, \frac{\partial g_r}{\partial x}(x, t_1|x_0, 0)|_{x=0} \tag{3.41}$$

Now, imagine that both the initial and final point are > 0, then we will have two class of possibilities of travelling between those two points: either we remain in the same side of x=0 (and thus we are in a "fully restricted path"' case), or we can also travel somewhere else in space, crossing x=0 one or many times, and coming back to reach our final point. Mathematically this means we have:

$$g(x_1, \tau|x_0, 0) = \frac{1}{2m} \int_0^\tau \mathrm{d}t_1\, g(x_1, \tau|0, t_1)\, \frac{\partial g_r}{\partial x}(x, t_1|x_0, 0)|_{x=0} + g_r(x_1, t|x_0, 0) \tag{3.42}$$

the second term of this equation is the fully restricted propagator that correspond to paths without crossing ("‘direct paths"’). It can be written, using the method of images:

$$g_r(x_1,\tau|x_0,0) = \theta(x_1)\theta(x_0)(g_f(x_1,\tau|x_0,0) - g_f(-x_1,\tau|x_0,0)) \tag{3.43}$$

with g_f the propagator fo the free particle

$$g_f(x_1,\tau|x_0,0) = \left(\frac{m}{i2\pi\tau}\right)^{1/2} exp(im(x_1-x_0)^2/2\tau) \tag{3.44}$$

as a result, we have:

$$\frac{\partial g_r}{\partial x}(x,t_1|x_0,0)|_{x=0} = 2\frac{\partial g_f}{\partial x}(0,t_1|x_0)\theta(x_0) \tag{3.45}$$

The propagator from x=0 to x=0 is given in [14]:

$$g(0,t|0,0) = \left(\frac{m}{i2\pi}\right)^{1/2} \frac{1-exp(-V_0 t)}{V_0 t^{3/2}} \tag{3.46}$$

the full solution will therefore have the form

$$\psi(x,\tau) = \theta(-x)\psi_{tr}(x,\tau) + \theta(x)(\psi_{ref}(x,\tau) + \psi_f(x,\tau)) \tag{3.47}$$

Here we have ψ_{tr}, transsmitted part of the wavefunction, ψ_{ref} the reflected part, and ψ_f the free part. the free part correspond to the portion of the wave packet that has not reached yet x=0 within the elapsed time $[0,\tau]$. Since, if we wait long enough, it is expected that all the wave packet crosses x=0, we can see that ψ_f goes to zero with large τ"

3.4 Example: scattering solutions of Schrödinger Equation

What we will do now is to calculate the scattering solutions of Schrödinger equation using PDX methods. One of our motivations for doing this, is that, once we will have derived these solutions, we will see that these solutions can be found within a certain approximation of semiclassical nature. By comparing the solutions obtained with PDX methods and those obtained with the semiclassical approximation, we will know what are the limits of validity of this approximation, and we will use it later in this work in our calculation of the arrival time distribution.

Let us assume that τ is large enough so that we can assume ψ_f to be zero. Starting with ψ_{tr}, we have:

$$\begin{aligned}\psi_{tr}(x,\tau) = \frac{1}{m^2}\int_0^{\tau} \mathrm{d}s \int_0^{\tau-s} \mathrm{d}v < x|exp(-iH_0 s)\hat{p}|0 > e^{-V_0 s} \\ . < 0|exp(-iHv)|0 >< 0|\hat{p}exp(-iH_0(\tau - v - s))|0 >\end{aligned} \tag{3.48}$$

where |0> is the position eigenstate at x=0, $s = \tau - t_1$ and v=$t_2 - t_1$, and H is just the total hamiltonian (free hamiltonian + complex potential). Then we decompose the initial state over momentum states |p>, and using $E = p^2/2m$:

$$\begin{aligned}\psi_{tr}(x,\tau) = \frac{1}{m^2}\int \mathrm{d}p \int_0^{\infty} \mathrm{d}s < x|exp(-iH_0 s)\hat{p}|0 > e^{i(E+iV_0)s} \\ . \int_0^{\infty} \mathrm{d}v < 0|exp(-iHv)|0 > \; e^{iEv}\, p \; < 0|p > e^{iE\tau}\psi(p)\end{aligned} \tag{3.49}$$

we need the following formula [17] to compute the above integral with respect to s:

$$\int_0^{\infty} \mathrm{d}s \left(\frac{m}{2\pi i s}\right)^{1/2} exp\left(i[\lambda s + \frac{mx^2}{2s}]\right) = \left(\frac{m}{2\lambda}\right)^{1/2} exp(i|x|\sqrt{2m\lambda}) \tag{3.50}$$

differentiating with respect to x and substituting $\lambda = E + iV_0$:

$$\int_0^{\infty} \mathrm{d}s < x|exp(-iH_0 s)\hat{p}|0 > e^{i(E+iV_0)s} = m\, exp(i|x|[2m(E + iV_0)]^{1/2}) \tag{3.51}$$

using then the formula

$$\left(\frac{m}{2\pi i}\right)^{1/2}\int_0^{\infty} \mathrm{d}v \frac{1 - e^{-V_0 v}}{V_0 v^{3/2}} e^{iEv} = \frac{\sqrt{2m}}{(E + iV_0)^{1/2} + E^{1/2}} \tag{3.52}$$

we can finally perform the integration of $\psi_{tr}(x,\tau)$ and get

$$\psi_{tr}(x,\tau) = \int \frac{\mathrm{d}p}{\sqrt{2\pi}} exp(-ix[2m(E + iV_0)]^{1/2} - iE\tau)\psi_{tr}(p) \tag{3.53}$$

where we have

$$\psi_{tr}(p) = \frac{2}{1 + E^{-1/2}(E + iV_0)^{1/2}}\psi(p) \tag{3.54}$$

The case of ψ_{ref} is different: because it corresponds to a portion of the wave packet that is reflected, it means that both points, initial and final, are of same side with respect to x=0, but with V_0 in the last segment of propagation. We obtain:

$$\psi_{ref}(x,\tau) = \int \frac{\mathrm{d}p}{\sqrt{2\pi}} exp(ixp - iE\tau)\psi_{ref}(p) \tag{3.55}$$

with

$$\begin{aligned}\psi_{ref}(p) &= \psi_{tr}(p) - \psi(p) \\ &= \frac{1 - E^{-1/2}(E + iV_0)^{1/2}}{1 + E^{-1/2}(E + iV_0)^{1/2}}\psi(p)\end{aligned} \tag{3.56}$$

Now that we have these exact result, we would like to test an approximation of the propagator based on the assumption we have a very small V_0 with respect to the energy scales, and write

$$< x|exp(-iHs)|0 > \approx < x|exp(-iH_0 s)|0 > exp(-V_0 s) \tag{3.57}$$

we will first calculate the transmitted wave packet:

$$\psi_{tr}(x,\tau) = -\frac{1}{m}\int_0^\tau \mathrm{d}s < x|e^{-iH_0 s}|0 > \; e^{-V_0 s} \; < 0|\hat{p}e^{-iH_0}(\tau - s)|\psi > \tag{3.58}$$

again here we have s= $\tau - t_1$. Then we take the limit for τ going to infinity and after this, we integrate. We then need to calculate

$$\int_0^\infty \mathrm{d}s < x|e^{-iH_0 s}|0 > \; e^{i(E+iV_0)s} = \left(\frac{m}{2(E + iV_0)}\right)^{1/2} exp(-ix[2m(E + iV_0)]^{1/2}) \tag{3.59}$$

which gives

$$\psi_{tr}(p) = \frac{1}{E^{-1/2}(E + iV_0)^{1/2}}\psi(p) \tag{3.60}$$

Comparing with the expression we obtained for $\psi_{tr}(p)$ with the PDX method, we see that the two answers are the same only when $V_0 = 0$, so we can infer that the approximation is valid for small V_0 with respect to the energy scale.

3.5 Classical case with a complex potential

We start with a classical phase space distribution $w_t(p,q)$ of initial $w_0(p,q)$ located in the region q>0 and with negative momenta. The evolution equation is

$$\frac{\partial w}{\partial t} = \frac{p}{m}\frac{\partial w}{\partial q} - 2V(q)w \tag{3.61}$$

where $V(q)$ is such that:

$$V(q) = V_0\theta(-q) \tag{3.62}$$

Solving the evolution equation, we get:

$$w_\tau(p,q) = exp\left(-2\int_0^\tau \mathrm{d}sV(q-ps/m)\right)w_0(p,q-p\tau/m) \tag{3.63}$$

and then doing like in the chapter 2, we find the probability

$$N(\tau) = \int_{-\infty}^{\infty}\mathrm{d}p\int_{-\infty}^{\infty}\mathrm{d}q\, w_\tau(p,q) \tag{3.64}$$

and we deduce the arrival time through a simple differentiation

$$\begin{aligned}\Pi(\tau) &= -\frac{dN}{d\tau}\\ &= 2V_0\int_{-\infty}^{\infty}\mathrm{d}p\int_{-\infty}^{\infty}\mathrm{d}q\, w_\tau(p,q)\end{aligned} \tag{3.65}$$

it appears that $\Pi(\tau)$ satisfies the equation

$$\frac{\mathrm{d}\Pi}{\mathrm{d}\tau} + 2V_0\Pi = -2V_0\int_{-\infty}^{\infty}\mathrm{d}p\frac{p}{m}w_\tau(p,0) \tag{3.66}$$

which has the solution

$$\Pi(\tau) = -2V_0\int_0^\tau \mathrm{d}texp(-2V_0(\tau-t))\int_{-\infty}^{\infty}\mathrm{d}p\frac{p}{m}w_\tau(p,0) \tag{3.67}$$

so we finally find

$$w_\tau(p,0) = e^{-2V_0\int_0^t \mathrm{d}s\theta(\frac{ps}{m})}w_0(p,\frac{-pt}{m}) \tag{3.68}$$

and thus

$$\Pi(\tau) = 2V_0\int_0^\tau \mathrm{d}t\, exp(-2V_0(\tau-t))\, J(t) \tag{3.69}$$

with

$$J(t) = -\int_{-\infty}^{\infty} \mathrm{d}p \frac{p}{m} w_0(p, \frac{-pt}{m}) \tag{3.70}$$

these last two equations are very important because this is what we obtain in the quantum case , in the section on the calculation of arrival time distribution.

Now, this classical result can help in shedding some light on the resolution function R, taht we have met in the chapter 2, it describes actually a sort of "'coarse graining in time"' (hence the name resolution function). To understand why, let us consider the prbability to arrive between τ_1 and τ_2. We have:

$$\begin{aligned} p(\tau_2, \tau_1) &= \int_{\tau_1}^{\tau_2} \mathrm{d}\tau \Pi(\tau) \\ &= 2V_0 \int_{\tau_1}^{\tau_2} \mathrm{d}\tau \int_0^{\tau} \mathrm{d}t\, exp(-2V_0(\tau - t))\, J(t) \end{aligned} \tag{3.71}$$

because we can reorder these integrals, we can write:

$$\begin{aligned} p(\tau_2, \tau_1) &= 2V_0 \int_0^{\tau_1} \mathrm{d}t \int_{\tau_1}^{\tau_2} \mathrm{d}\tau exp(-2V_0(\tau - t))\, J(t) \\ &+ 2V_0 \int_{\tau_1}^{\tau_2} \mathrm{d}t \int_t^{\tau_2} \mathrm{d}\tau exp(-2V_0(\tau - t))\, J(t) \\ &= \int_0^{\tau_1} \mathrm{d}t\, (exp(-2V_0(\tau_1 - t)) - exp(-2V_0(\tau_2 - t)))\, J(t) \\ &+ \int_{\tau_1}^{\tau_2} \mathrm{d}t (1 - exp(-2V_0(\tau_2 - t))) J(t) \end{aligned} \tag{3.72}$$

Now, in this formula, we see that if we could, in some way, neglect the exponential terms, the expression would greatly simplify and just be $\int dtJ$. For this to happen, we need the argument of the exponential to be very big, that is, $V_0\tau >> 1$, which implies a relation between τ and V_0, namely, that the timescales are much greater than V_0

$$p(\tau_2, \tau_1) \approx \int_{\tau_1}^{\tau_2} \mathrm{d}t\, J(t) \tag{3.73}$$

3.6 the arrival time distribution

We would like to calculate the following expression

$$\Pi(\tau) = 2V_0 < \psi_\tau|\theta(-\hat{x})|\psi_\tau > \tag{3.74}$$

where we have

$$\begin{aligned} |\psi_\tau > &= exp(-iH\tau)|\psi > \\ &= exp(-iH_0\tau - V_0\theta(-\hat{x})\tau)|\psi > \end{aligned} \tag{3.75}$$

We will be interested in the regime of small V_0, which will allow us to use the semiclassical approximation we have talked earlier.

Using the PDX formula involving first crossing, we can write:

$$< x|exp(-iH\tau)|\psi >= -\frac{1}{m}\int_0^\tau \mathrm{d}t < x|exp(-iH(\tau-t))\delta(\hat{x})\hat{p}exp(-iH_0t)|\psi > \tag{3.76}$$

using the fact that $\delta(\hat{x})$ has the following property (for any operator A):

$$\delta(\hat{x})A\delta(\hat{x}) = \delta(\hat{x}) < 0|A|0 > \tag{3.77}$$

we obtain then (again writing $s = \tau - t$, $s' = \tau - t'$

$$\begin{aligned} \Pi(\tau) = \frac{2V_0}{m^2}&\int_0^\tau \mathrm{d}s' \int_0^\tau \mathrm{d}s \int_{-\infty}^0 \mathrm{d}x \\ .& < 0|exp(iH^+s')|x >< x|exp(-iHs)|0 > \\ .& < \psi|exp(iH_0(\tau-s'))\,\hat{p}\,\delta(\hat{x})\,\hat{p}\,exp(iH_0(\tau-s))|\psi > \end{aligned} \tag{3.78}$$

This relabelling of our integrals will make things easier to be computed. We start with the dx-integral, and we use here the semiclassical approximation we had mentioned before:

$$< x|exp(-iHs)|0 >\approx \left(\frac{m}{2\pi is}\right)^{1/2} exp(\frac{imx^2}{2s} - V_0s) \tag{3.79}$$

which gives us after integration:

$$\begin{aligned} \Pi(\tau) = \frac{V_0}{m^2}\int_0^\tau \mathrm{d}s' \int_0^\tau \mathrm{d}s \left(\frac{m}{2\pi i}\right)^{1/2} \frac{e^{-V_0(s+s')}}{(s-s')^{1/2}} \\ . < \psi_\tau|exp(-iH_0s')\,\hat{p}\,\delta(\hat{x})\,\hat{p}\,exp(iH_0s)|\psi_\tau > \end{aligned} \tag{3.80}$$

Now, let us have a look to the two ds/ds′ integrals. Geometrically, we can see that

$$\int_0^\tau \mathrm{d}s' \int_0^\tau \mathrm{d}s = \int_0^\tau \mathrm{d}s' \int_{s'}^\tau \mathrm{d}s + \int_0^\tau \mathrm{d}s \int_s^\tau \mathrm{d}s' \tag{3.81}$$

performing then the relabelling u=s′,v=s-s′ in the first integral, and u=s,v=s-s′ in the second one, we get

$$\begin{aligned}\Pi(\tau) &= \frac{V_0}{m^2}\left(\frac{m}{2\pi}\right)^{1/2} \int_0^\tau \mathrm{d}u e^{-2V_0 u} \int_0^{\tau-u} \mathrm{d}v \frac{e^{-V_0 v}}{v^{1/2}} \\ &.(\frac{1}{\sqrt{i}} < \psi_\tau | exp(-iH_0 u)\, \hat{p}\, \delta(\hat{x})\, \hat{p}\, exp(iH_0(u+v)) | \psi_\tau > \\ &+ \frac{1}{\sqrt{-i}} < \psi_\tau | exp(-iH_0(u+v))\, \hat{p}\, \delta(\hat{x})\, \hat{p}\, exp(iH_0 u) | \psi_\tau >)\end{aligned} \tag{3.82}$$

the final result is

$$\begin{aligned}\Pi(\tau) &= 2V_0 \int_0^\tau \mathrm{d}u\, e^{-2V_0 u} \\ &\cdot \frac{1}{2m} < \psi_{\tau-u} | \hat{p}\, \delta(\hat{x}) \Sigma(\hat{p}) + \Sigma^+(\hat{p}) \delta(\hat{x})\, \hat{p} | \psi_{\tau-u} >\end{aligned} \tag{3.83}$$

here $\Sigma(\hat{p})$ is

$$\Sigma(\hat{p}) = \frac{\hat{p}}{[2m(H_0 + iV_0)]^{1/2}} \tag{3.84}$$

and if V_0 is very small

$$\Sigma(\hat{p}) \approx \hat{p}/|\hat{p}| \tag{3.85}$$

so that sigma is in fact just a sign function of the momentum. Now, if we write $u = \tau - t$, we find

$$\begin{aligned}\Pi(\tau) &= 2V_0 \int_0^\tau \mathrm{d}t\, e^{-2V_0(\tau - t)} \frac{-1}{2m} < \psi_t | \hat{p}\, \delta(\hat{x}) + \delta(\hat{x})\, \hat{p} | \psi_t > \\ &= 2V_0 \int_0^\tau \mathrm{d}t\, e^{-2V_0(\tau-t)} J(t)\end{aligned} \tag{3.86}$$

which is exactly what we obtained classically (the only difference being the range of integration)!!

Chapter 4

Decoherence of histories

4.1 Introduction to the concept of decoherent histories

The purpose of this section is to introduce what we call the decoherent histories approach to the arival problem.

The fundamental tools we use to describe a "'history"' are probabilities defined such that

$$p(\alpha_1, \alpha_2, \alpha_3, ...) = Tr(C_{\underline{\alpha}} \rho C^{\dagger}_{\underline{\alpha}}) \tag{4.1}$$

here the $C_{\underline{\alpha}}$ are class operators, which are time ordered chains of projectors:

$$C_{\underline{\alpha}} = P_{\alpha n}\, e^{-iH(t_n - t_{n-1})} ... e^{-iH(t_2 - t_1)} P_{\alpha 1} \tag{4.2}$$

The class operators are such that:

$$\sum_{\underline{\alpha}} C_{\underline{\alpha}} = e^{-iH\tau} \tag{4.3}$$

where $\tau = [t_1, t_n]$.

Such histories can sometimes "'interfer"' and we describe this interference with what is named a decoherence functional:

$$D(\underline{\alpha}, \underline{\alpha}') = Tr(C_{\underline{\alpha}} \rho C^{\dagger}_{\underline{\alpha}'}) \tag{4.4}$$

Decoherence functionals satisfy the three following identities:

$$D(\underline{\alpha}, \underline{\alpha}') = D * (\underline{\alpha}', \underline{\alpha}) \tag{4.5}$$

$$\sum_{\underline{\alpha},\underline{\alpha}'} D(\underline{\alpha},\underline{\alpha}') = 1 \tag{4.6}$$

$$\sum_{\underline{\alpha}} D(\underline{\alpha},\underline{\alpha}) = \sum_{\underline{\alpha}} p(\underline{\alpha}) = 1 \tag{4.7}$$

Now, if histories don't interfer, the decoherence function is zero:

$$D(\underline{\alpha},\underline{\alpha}') = 0 \Leftrightarrow (\underline{\alpha} \neq \underline{\alpha}') \tag{4.8}$$

It is generally not easy to have situations where the decoherence are exactly zero, also, we are interested in knowing when we can indeed considering D as a negligible quantity. A hint is provided by the following relation [18]

$$|D(\underline{\alpha},\underline{\alpha}')|^2 \leq p(\underline{\alpha})p(\underline{\alpha}') \tag{4.9}$$

which allows us to decide that we will consider histories to be decoherent if we have

$$|D(\underline{\alpha},\underline{\alpha}')|^2 << p(\underline{\alpha})p(\underline{\alpha}') \tag{4.10}$$

Now, in addition to probabilities, we can also define quasi-probabilities. They are of the form:

$$q(\underline{\alpha}) = Tr(C_{\underline{\alpha}}\rho e^{iH\tau}) \tag{4.11}$$

It is straightforward to see that

$$\begin{aligned} q(\underline{\alpha}) &= \sum_{\underline{\alpha}'} Tr(C_{\underline{\alpha}}\rho C^{\dagger}_{\underline{\alpha}'}) \\ &= p(\underline{\alpha}) + \sum_{\underline{\alpha}' \neq \underline{\alpha}'} D(\underline{\alpha},\underline{\alpha}') \end{aligned} \tag{4.12}$$

So, when we have decoherence, then quasi-probabilities and probabilities are equal. However in the most general case it is not necessarily the case, as quasi-probabilities can be negative, or even imaginary.

Our aim now is to manage to describe arrival time in terms of these new concepts. We will need for this some more precise expressions and definitions of the class operators. We will use two class operators, that will corresponds to the two types of histories we can get: either crossing x=0 or not crossing it. A possible definition for the "'not crossing"' class operator could be

$$C_{nc} = lim_{\epsilon \to 0} Pe^{-iH\epsilon}P...e^{-iH\epsilon}P \tag{4.13}$$

which takes, in the continuous limit, the form of the restricted operator we have already met:

$$C_{nc} = g_r(\tau, 0) \tag{4.14}$$

which itself relates to the path integral:

$$< x_1|g_r(\tau, 0)|x_0 >= \int_r \mathcal{D}xe^{iS} \tag{4.15}$$

we can then deduce the "'crossing"' class operator:

$$C_c = e^{-iH\tau} - C_{nc} \tag{4.16}$$

There is, however, a problem with our C_{nc}: it is subject to the Zeno effect, that is, too many projections will generate a total reflection, and this leads that x=0 is never crossed, that is,

$$p_{nc} = Tr(C_{nc}\rho C_{nc}^{\dagger}) \tag{4.17}$$

a possible way to get rid of this problem is either to avoid taking the limit as we did, ot chosing a more suitable operator (by taking for example POVM's instead of projectors). What we will do is a mix of both. First, we will not take the limit, and simply work with

$$C_{nc}^{\epsilon} = Pe^{-iH\epsilon}P...e^{-iH\epsilon}P \tag{4.18}$$

it can then be proven that Zeno effect can be avoided if

$$\epsilon > \frac{1}{\Delta H_0} \tag{4.19}$$

Then, following a result of Echanobe al. [19], we will use the following approximation

$$Pe^{-iH\epsilon}P...e^{-iH\epsilon}P \approx e^{-iH_0\tau - V_0\theta(-\hat{x})\tau} \tag{4.20}$$

this approximation is based on the fact that we can write

$$P = \theta(\hat{x}) \approx exp(-V_0\theta(-\hat{x})\epsilon) \tag{4.21}$$

when

$$V_0\epsilon >> 1 \tag{4.22}$$

On another hand, we have similarly

$$exp(-iH_0\epsilon)exp(-V_0\theta(-\hat{x})\epsilon) \approx (-iH_0\epsilon - V_0\theta(-\hat{x})\epsilon) \tag{4.23}$$

under the condition

$$V_0\epsilon^2| < [H_0, \theta(-\hat{x})] > | << 1 \tag{4.24}$$

assuming that

$$V_0 >> \Delta H_0 \tag{4.25}$$

We then have finally an interesting form for our not-crossing class operator:

$$C_{nc} = exp(-iH_0\tau - V_0\theta(-\hat{x})\tau) \tag{4.26}$$

what we will show in the subsequent sections is that the class operator for crossing takes the form

$$\begin{aligned} C_c^k &= e^{-iH_0\tau}\int_{t_k}^{t_{k+1}} \mathrm{d}t\frac{-1}{2m}(\hat{p}\delta(\hat{x}_t) + \delta(\hat{x}_t)\hat{p}) \\ &= e^{-iH_0\tau}(\theta(\hat{x}(t_k)) - \theta(\hat{x}(t_{k+1}))) \end{aligned} \tag{4.27}$$

and that, if decoherence is satisfied, the (quasi)probabilities take the form

$$q(t_k, t_{k+1}) = \int_{t_k}^{t_{k+1}} \mathrm{d}t\, J(t) \tag{4.28}$$

which completely agrees all result shown in other chapters.

4.2 single large time interval analysis

Let us suppose we have a wave packet going to the origin from positive x's. We are looking for the probability to cross te origin during a time interval.

We know that the not-crossing and crossing class operators are given by

$$C_{nc} = exp(-iH_0\tau - V(x)\tau) \tag{4.29}$$

$$C_c = exp(-iH_0\tau) - exp(-iH_0\tau - V(x)\tau) \tag{4.30}$$

and the sum of them satisfies

$$C_{nc} + C_C = e^{-iH_0\tau} \tag{4.31}$$

we want to calculate the two probabilities

$$p_{nc}(\tau) = Tr(C_{nc}\rho C_{nc}^{+}) \tag{4.32}$$

$$p_c(\tau) = Tr(C_c\rho C_c^{+}) \tag{4.33}$$

and the off-diagonal components of the decoherence functional:

$$\begin{aligned} D_{c,nc} &= Tr(C_{nc}\rho C_c^{+}) \\ &= Tr(C_{nc}\rho e^{-iH_0\tau}) - p_{nc} \end{aligned} \tag{4.34}$$

it is straightforward to see that

$$p_{nc} + p_c + D_{c,nc} + D^{*}_{c,nc} = 1 \tag{4.35}$$

We have to remember that the interesting situations are those where we have decoherence:

$$D_{c,nc} = 0 \tag{4.36}$$

because then we obtain a simple sum rule for the probabilities:

$$p_{nc}(\tau) + p_c(\tau) = 1 \tag{4.37}$$

Now, if we notice that p_{nc} is nothing else than the survival probability N, we can immediatly see that

$$p_{nc}(\tau) = 1 + \int_0^{\tau} \mathrm{d}t \, \frac{\mathrm{d}p_{nc}}{\mathrm{d}t} \tag{4.38}$$

and thus

$$p_{nc}(\tau) = 1 - \int_0^\tau \mathrm{d}t\Pi(t) \tag{4.39}$$

which, when there is decoherence, just allow us to write

$$p_c(\tau) = \int_0^\tau \mathrm{d}t\Pi(t) \tag{4.40}$$

We will now carry a careful calculation of the decoherence functional in the case of a single large interval $[0, \tau]$. Let us remember that we have seen previously the expressions for the transmitted and reflected wave packet, and using them, we have that:

$$C_{nc}|\psi >= \theta(-\hat{x})|\psi_{tr} > +\theta(\hat{x})(|\psi_{ref} > +|\psi_f >) \tag{4.41}$$

$$C_c|\psi >= \theta(-\hat{x})(|\psi_f > -|\psi_{tr} >) - \theta(\hat{x})|\psi_{ref} > \tag{4.42}$$

so that the probabilities and off-diagonal terms of the decoherence functional are

$$\begin{aligned} p_{nc} &=< \psi_{tr}|\psi_{tr} > + < \psi_{ref}|\psi_{ref>} + < \psi_{ref}|\psi_f > + < \psi_f|\theta(\hat{x})|\psi_f > \\ p_c &=< \psi_{tr}|\psi_{tr} > + < \psi_{ref}|\psi_{ref} > - < \psi_{tr}|\psi_f > - < \psi_f|\psi_{tr} > - < \psi_f|\theta(\hat{x})|\psi_f > \\ D_{c,nc} &=< \psi_{tr}|\psi_f > - < \psi_{tr}|\psi_{tr} > - < \psi_{ref}|\psi_{ref} > - < \psi_f|\psi_{ref} > \end{aligned} \tag{4.43}$$

Now, what we will do is to use the quasi-probability for not-crossing

$$q_{nc}(\tau) = Tr(C_{nc}\rho e^{-iH_0\tau}) \tag{4.44}$$

and we know that the difference between the quasi-probability and the probability is just the decoherence functional:

$$D_{c,nc} = q_{nc}(\tau) - p_{nc}(\tau) \tag{4.45}$$

So, the most intuitive way to see if there is decoherence is to see if p and q are the same or not. This is basically the direction of reasoning we will follow, however we will write our equations in a more suggestive way. For this, we write:

$$q_{nc}(\tau) = 1 + \int_0^\tau \mathrm{d}t\, \frac{\mathrm{d}q_{nc}}{\mathrm{d}t} \tag{4.46}$$

and name

$$\tilde{\Pi}(t) \equiv \frac{\mathrm{d}q_{nc}}{\mathrm{d}t} \tag{4.47}$$

we have thus

$$q_{nc}(\tau) = 1 + \int_0^\tau \mathrm{d}t\, \tilde{\Pi}(t) \tag{4.48}$$

and the decoherence functional becomes simply

$$D_{c,nc} = \int_0^\tau \mathrm{d}t\, (\Pi(t) - \tilde{\Pi}(t)) \tag{4.49}$$

now, the explicit expression for $\tilde{\Pi}$ is

$$\tilde{\Pi}(t) = V_0 < \psi|exp(iH_0t)\theta(-\hat{x})exp(-iH_0t - V_0\theta(-\hat{x})t)|\psi > \tag{4.50}$$

but we have seen how to solve this type of equation in the previous chapter, and we get finally

$$\tilde{\Pi}(t) = V_0 \int_0^t \mathrm{d}s\, e^{-V_0(\tau - s)} J(s) \tag{4.51}$$

we can also calculate that

$$\int_0^\tau \mathrm{d}t\, \Pi(t) \approx \int_0^\tau \mathrm{d}t\, J(t) \tag{4.52}$$

We musnt't forget that all these calculations are carried under the semiclassical approximation we mentioned in the previous chapter, which is itself valid if V_0 is very small,and that, as the same time, we are here in the hypothesis of a single large time interval, so that Π and $\tilde{\Pi}$ give the same result, that is, the decoherence functional vanish. This shows that the hypothesis that describe the study of the arrival time problem we carried in the previous chapter corresponds to situation where decoherence is satisfied, at least in the case of a single large interval. We will now study the more complex case of an arbitrary set of time intervals.

4.3 Arbitrary set of time interval analysis

The idea here to split the overall time interval we are considering $[0;\tau]$ into small infinitesimal times dt's, during each of which we are interested to know whether the particle has crossed. In order to do that, we will write, like we dit many times,$\tau = \epsilon.n$. Like we had so far, we can obviously write:

$$e^{-iH_0\epsilon} = C_{nc}(\epsilon) + C_c(\epsilon) \tag{4.53}$$

Since $\tau = \epsilon.n$, we have then

$$\begin{aligned} e^{-iH_0\tau} &= (e^{-iH_0\epsilon})^n \\ &= (e^{-iH_0\epsilon})^{n-1}(C_{nc}(\epsilon) + C_c(\epsilon)) \\ &= (e^{-iH_0\epsilon})^{n-1}C_{nc}(\epsilon) + e^{-iH_0(\tau-\epsilon)}C_c(\epsilon) \end{aligned} \tag{4.54}$$

repeating this same steps in the first term, we have

$$e^{-iH_0\tau} = (e^{-iH_0\epsilon})^{n-2}C_{nc}(2\epsilon) + e^{-iH_0(\tau-2\epsilon)}C_c(\epsilon)C_{nc}(\epsilon) + e^{-iH_0(\tau-\epsilon)}C_c(\epsilon) \tag{4.55}$$

by iterating the process:

$$e^{-iH_0\tau} = C_{nc}(\tau) + \sum_{k=0}^{n-1} e^{-iH_0(\tau-(k+1)\epsilon)}C_c(\epsilon)C_{nc}(k\epsilon) \tag{4.56}$$

As a result, we see that the probability to cross x=0 the first time during $[k\epsilon, (k+1)\epsilon]$ is just

$$C_c((k+1)\epsilon, k\epsilon) = e^{-iH_0(\tau-(k+1)\epsilon)}C_c(\epsilon)C_{nc}(k\epsilon) \tag{4.57}$$

Now, we take the continuum limit of $e^{-iH_0\tau}$ and insert the expression for C_{nc}:

$$e^{-iH_0\tau} = e^{-iH_0\tau - V\tau} + \int_0^\tau \mathrm{d}t\, e^{-iH_0(\tau-t)}Ve^{-iH_0t-Vt} \tag{4.58}$$

the probability for first crossing during [t,t+dt] will be

$$C_c(t) = e^{-iH_0(\tau-t)}V\, e^{-iH_0t-Vt} \tag{4.59}$$

however, since there is no reason to think there will be no decoherence, we consider the more general "‘coarse-grained"’ expression

$$C_c^k = \int_{t_k}^{t_{k+1}} \mathrm{d}t\, C_c(t) \tag{4.60}$$

as a result, the overall number of class operators will be N+1: one for not crossing, and N for a possibility of crossing at each of the N intervals that we called epsilons:

$$C_\alpha = \left\{C_{nc}, C_c^k\right\} \tag{4.61}$$

and they must all satisfy, like usual:

$$e^{-iH_0\tau} = C_{nc} + \sum_{k=0}^{N-1} C_c^k \tag{4.62}$$

The decoherence here will be more tricky because now we have two types of relations to check:

$$D_{kk'} = Tr(C_c^k \rho (C_c^{k'})^+) \tag{4.63}$$

and

$$D_{k,nc} = Tr(C_c^k \rho (C_{nc})^+) \tag{4.64}$$

Now, what we will do is to write in a simpler way the class operator that describes the crossing. We start with

$$< x|e^{iH_0\tau} C_c(t)|\psi > = V_0 \ < x|e^{iH_0 t} \theta(-\hat{x}) e^{-iH_0 t - Vt}|\psi > \tag{4.65}$$

by doing exactly the same type of calculation that what we did when we computer the arrival time distribution in the previous chapter, we find that

$$< x|e^{iH_0\tau} C_c(t)|\psi > = V_0 \int_0^t \mathrm{d}s\, e^{-V_0(t-s)} \frac{-1}{2m} \ < x|(\hat{p}\delta(\hat{x}_s) + \delta(\hat{x}_s)\hat{p})|\psi > \tag{4.66}$$

with similar hypothesis, that is, V_0 much smaller than energy scales. After interating over time, we get

$$e^{iH_0\tau} C_c^k = \int_{t_k}^{t_{k+1}} \mathrm{d}t\, \frac{-1}{2m} (\hat{p}\delta(\hat{x}_t) + \delta(\hat{x}_t)\hat{p}) \tag{4.67}$$

which can elegantly take the form

$$e^{iH_0\tau} C_c^k = \theta(\hat{x}(t_k)) - \theta(\hat{x}(t_{k+1})) \tag{4.68}$$

We are now ready to compute the probability for crossing. It is

$$p(t_k, t_{k+1}) = Tr(C_c^k \rho (C_c^k)^+) \tag{4.69}$$

which becomes in the case of decoherence

$$
\begin{aligned}
p(t_k, t_{k+1}) &= Tr(C_c^k \rho e^{iH_0\tau}) \\
&= \int_{t_k}^{t_{k+1}} \mathrm{d}t \, \frac{-1}{2m} \, < \psi|(\hat{p}\delta(\hat{x}_t) + \delta(\hat{x}_t)\hat{p})|\psi > \\
&= \int_{t_k}^{t_{k+1}} \mathrm{d}t \, J(t)
\end{aligned}
\tag{4.70}
$$

and this matches exactly all our previous results!

4.4 Decoherence and backflow

In this section we would like to adress an important question which is the relation between backflow and decoherence. We consider in a simple approach, histories that either cross or don't during a certain time interval. If crossing is just written C, then the not crossing operator can be written just 1-C, with

$$C = \theta(\hat{x}_1) - \theta(\hat{x}_2) \tag{4.71}$$

where we focus on the meaning here, and not really on technical aspect like the exponential, etc, which have no importance for what we want to explain.

We can calculate the decoherence functional:

$$
\begin{aligned}
D &=< C(1-C) > \\
&=< C > - < C^2 >
\end{aligned}
\tag{4.72}
$$

or, written differently:

$$C = - < \theta(-\hat{x}_1)\theta(\hat{x}_2) + \theta(\hat{x}_2)\theta(-\hat{x}_1) > \tag{4.73}$$

Having decoherence means having D=0, that is:

$$p(t_1, t_2) =< C^2 >=< C > \tag{4.74}$$

So what does it mean? When we have decoherence, $<C^2 > and < C > mustbeequal, but < C^2 > beingpositive, thismeansthat < C > ispositiveaswell.Nowletusimaginewehavebackflow.Then < C > isnegative, butifitisnegative, itcannotcancel < C^2 >, andtherecannotbedecoherence!So, animportantresul$

Chapter 5

The backflow problem

5.1 Introduction

The backflow effect is a physical process where we hve a negative current despite having positive momenta. It is an actual quantum phenomenon, despite the fact that we can show that, suprisingly, it does not depend on Planck's constant, unlike many quantum effects. Being a quantum process, it is expressed through the behavior of the probability density. Explicitly, , if we have a wave function located in the negative x-region, and propagating toward the positive x's,it appears that the probability of staying in the negative x's region increases with time, under certain conditions that we will develop in the following pages. What we can say already is that this backflow can be described by some quantities that some authors suggest to correspond to new quantum number, and it seems that the increase of the probability with time is bounded. This has been, and is still now, intensively explored, mainly through numerical work, and, when possible, analytically.

The problem can be expressed mathematically as follows. We start with a wave function located in x<0, and with positive momenta, as we just said. By "'located in x<0"' it should be understood "'centred in the negative region"'. Then, the amount of probability flux F that crosses the origin during a time interval is given by

$$
\begin{aligned}
F(t_1, t_2) &= \int_{-\infty}^{0} \mathrm{d}x\, |\psi(x, t_1)|^2 - \int_{-\infty}^{0} \mathrm{d}x\, |\psi(x, t_2)|^2 \\
&= \int_{t_1}^{t_2} \mathrm{d}t\, J(t)
\end{aligned}
\tag{5.1}
$$

with the familiar current at x=0:

$$J(t) = -\frac{i\hbar}{2m}\left(\psi^*(0,t)\frac{\partial\psi(0,t)}{\partial x} - \frac{\partial\psi^*(0,t)}{\partial x}\psi(0,t)\right) \tag{5.2}$$

as we have seen many times in the early sections of the second chapter, this flux can be written

$$F(t_1,t_2) = \int_{t_1}^{t_2} \mathrm{d}t \int \mathrm{d}p\mathrm{d}q \frac{p}{m}\delta(q)W_t(p,q) \tag{5.3}$$

what we will do now it to rewrite this flux in operator form. The motivation for this is that we would like to study the backflow effect by trying to setting up a eigenvalue problem, which would considerably makes things simpler. So, to write these formula in operator form, we use the projector $P = \theta(\hat{x})$, projecting on the positive x's, and its complement $\bar{P} = 1 - P = \theta(-\hat{x})$. We have then the flux operator $\tilde{F}(t_1,t_2)$

$$\begin{aligned}\tilde{F}(t_1,t_2) &= P(t_2) - P(t_1) \\ &= \int_{t_1}^{t_2} \mathrm{d}t\,\dot{P}(t) \\ &= \int_{t_1}^{t_2} \mathrm{d}t\,\frac{i}{\hbar}[H,\theta(\hat{x})] \\ &= \int_{t_1}^{t_2} \mathrm{d}t\,\hat{J}(t)\end{aligned} \tag{5.4}$$

with the current opetator, that we have also met many times previously in this dissertation:

$$\hat{J}(t) = \frac{1}{2m}(\hat{p}\delta(\hat{x}) + \delta(\hat{x})\hat{p}) \tag{5.5}$$

we have thus

$$\begin{aligned}F(t_1,t_2) &=< \hat{F}(t_1,t_2) > \\ &=< \bar{P}(t_1) > - < \bar{P}(t_2) > \\ &=< P(t_2) > - < P(t_1) > \\ &= \int_{t_1}^{t_2} \mathrm{d}t\ < \psi|\hat{J}(t)|\psi >\end{aligned} \tag{5.6}$$

with J(t)=$< \psi|\hat{J}(t)|\psi >$

it is worth to wonder under which condition this flux can possibly be negative for certain states. A first possibility is that it can happen when the function W itself is negative. This answer is quite intuitive indeed, but the integral that expresses F in terms of W can sometimes be positive even for negative W, so this condition, if it happens seems to happen along with another cause. Another possibility may come from the exploration of the current operator, where a negative $\hat{J}$ may be caused by teh non-commutativity of $\delta(\hat{x})$ and $\hat{p}$.

At this stage, we are ready for the eigenvalue problem, and the corresponding equation will be given by

$$\theta(\hat{p})\hat{F}(t_1, t_2)|\Phi >= \lambda|\Phi > \tag{5.7}$$

In this equation, backflow will correspond to states $|\Phi >$ of positive momenta, and with negative eigenvalues λ. For convenience, we will write the time interval [-T/2,T/2] instead of $F(t_1, t_2)$, so that we will have a single time quantity T.Also, because we would like to see explicitly in our equation that we are working with positive momenta, it is a good idea to switch our equation to momentum space. Positive momenta will then obviously correspond to a range of integration that go from zero to infinity, and we will thus have

$$\frac{1}{\pi}\int_0^\infty \mathrm{d}k \, \frac{sin[(p^2 - k^2)T/4m\hbar]}{p - k}\Phi(k) = \lambda\Phi(p) \tag{5.8}$$

a further good idea is to do a rescaling through the change of variables $p = 2\sqrt{m\hbar T}u$ and $k = 2\sqrt{m\hbar T}v$, and our equation then reads

$$\frac{1}{\pi}\int_0^\infty \mathrm{d}v \, \frac{sin(u^2 - v^2)}{u - v}\Phi(v) = \lambda\Phi(u) \tag{5.9}$$

with $\Phi(u) = (m\hbar/4T)^{1/4}\Phi(p)$ dimensionless. A critically important thing to notice is that, at the light of all these change of variable, it appears that the eigenvalue λ is in fact dimensionless.

In terms of these change of variables, we can also write the flux:

$$F(-T/2, T/2) = \frac{1}{\pi}\int_0^\infty \mathrm{d}u \int_0^\infty \mathrm{d}v \, \phi^*(u)\, \frac{sin(u^2 - v^2)}{u - v}\phi(v) \tag{5.10}$$

Since the eigenvalue equation is real, we expect the eigenfunctions to be real as well, so we should have:

$$\psi^*(x, t) = \psi(-x, -t) \tag{5.11}$$

and it appears that the numerical solutions of this eigenvalue equation is described with the interval

$$-c_{bm} \leq \lambda \leq 1 \tag{5.12}$$

here, c_{bm} is a number that has the same dimension than λ, meaning, it is dimensionless, and in particular, because of the change of variable we performed above, it does not depend on $\hbar$, which is at first unexpected. This special number has been explored intensively by Bracken and Melloy [20],[21],[22](hence the name of this number), and it seems to be a constant of value

$$c_{bm} \approx 0.0384 \tag{5.13}$$

Now, another thing that appears agin from the change of variable we did, is that this number does not depend on T either. as a result, a period of negative current can be arbitrarily long, as long as we still have

$$\int_{-T/2}^{T/2} \mathrm{d}t\, J(t) \geq -c_{bm} \tag{5.14}$$

which implies a relationship

$$T\, J(\xi) \geq -c_{bm} \tag{5.15}$$

for a certain $\xi \in$ [-T/2,T/2]

5.2 superposition of gaussians

In this section, we would like to review the study that has been carried [23] regarding the amount of backflow effect that can be obtained from superposition of gaussians. First, the reason why we straight consider superposition of gaussian rather than a single one, is that a single gaussian have necessarily a positive current, because its function W is positive. Now, regarding the case of superposition of gaussians, we know that there is a negative current contribution that comes from the wavepackets themselves, and this has of course nothing to do with backflow. It will be worth to see then what is the exact proportion of this geometry-related negative current with respect to the backflow itself. To make equations simpler, we will set $\hbar = 1$ and m=1

We start with the state

$$\psi'(x,t) = \sum_{k=1,2} A_k \, exp[i\, p_k(x - p_k t)] \tag{5.16}$$

with the A_k's are real. The current at the origin will be

$$J(t) = A_1^2 p_1 + A_2^2 p_2 + A_1 A_2 (p_1 + p_2) cos[(E_1 - E_2)t] \tag{5.17}$$

The *cos* function generates an oscillation between $(\mathrm{A}_1 p_1 + A_2 p_2)(A_1 + A_2) as maximum and (\mathrm{A}_1 p_1 - A_2 p_2)(A_1 - A_2)$ as minimum. Therefore we will have backflow for many values that are easy to deduce, for example from the minimum of the oscillation.

What we will do now is to consider the sum of two initially gaussian wavepackets of equal with σ:

$$\psi(x,t) = \sum_{k=1,2} A_k \frac{1}{\sqrt{4\sigma^2 + 2it}} exp\left(i\, p_k(x - p_k t) - \frac{(x - p_k t)^2}{4\sigma^2 + 2it} \right) \tag{5.18}$$

Let us have a look to some parameters and the corresponding plots taken from [23]: for the following set of parameters

$$\begin{aligned} p_1 &= 0.5 \\ p_2 &= 2 \\ \sigma &= 10 \\ A_1 &= 1.7 \\ A_2 &= 1 \end{aligned} \tag{5.19}$$

we clearly see that the plot of the current reveals intervals where this current is negative:

and plotting the probability for remaining in x<0 reveals that despite the fact that this probability decreases, it has some local increases with time:

The same type of phenomena can be obtained with other set of parameters, for example

$$\begin{aligned} p_1 &= 0.3 \\ p_2 &= 1.4 \\ \sigma &= 10 \\ A_1 &= 1.8 \\ A_2 &= 1 \end{aligned} \tag{5.20}$$

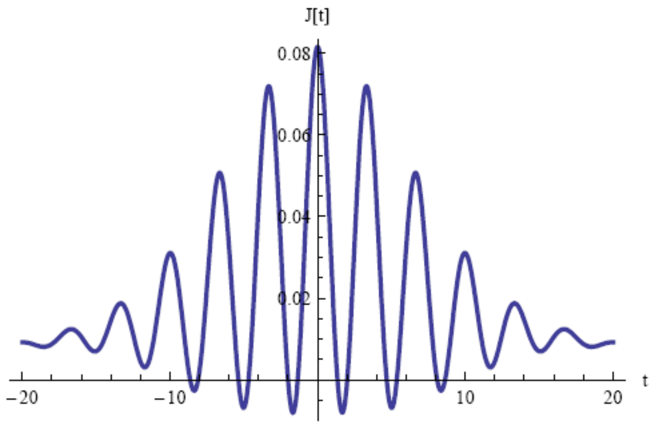

Figure 5.1:

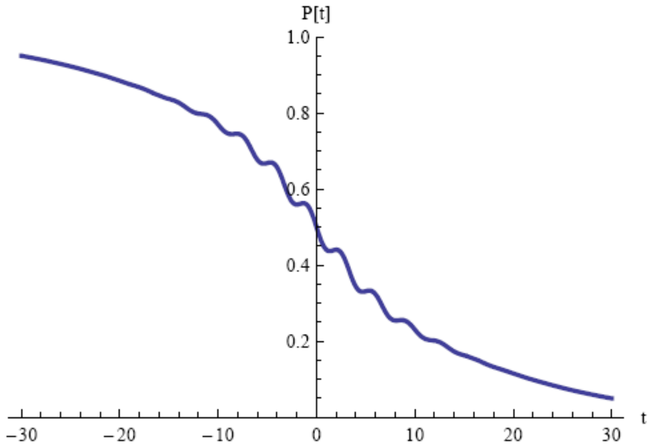

Figure 5.2:

where again we see intervals of negative current:
and intervals of increasing probability of remaining in the negative region:
from all this, we can try to calculate the largest period of backflow:

$$F = \int_{t_1}^{t_2} \mathrm{d}t\, J(t) \tag{5.21}$$

and we find

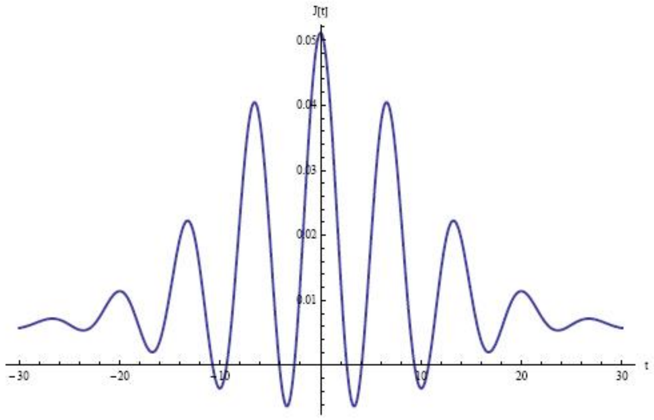

Figure 5.3:

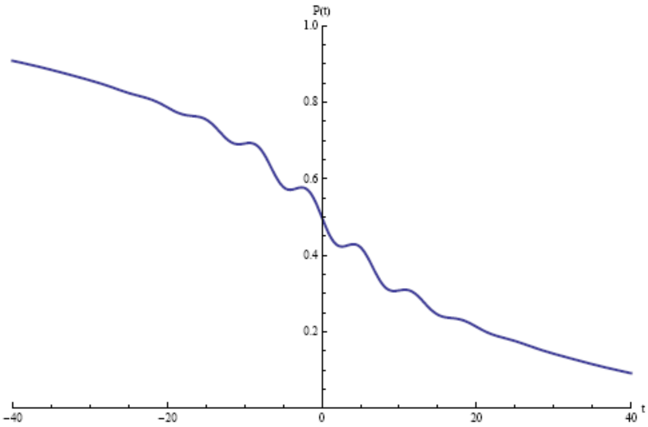

Figure 5.4:

$$F \approx -0.0061 \tag{5.22}$$

which is indeed very small. Now, as we have said in the beginning of this section, we should make sure that this negative current is not caused by the gaussian-geometry of the wavepacket. In fact, we can calculate, for example, that for the wavepacket centered around p=0.3, the associated probability to have a negative current will be

$$\begin{aligned}\text{Probability}(p < 0) &\approx \int_{-\infty}^{0} \mathrm{d}p\, exp(-200(p-0.3)^2) \\ &\approx 10^{-10}\end{aligned} \tag{5.23}$$

this is ridiculously small, and we can therefore infer that indeed our negative current is essentialy caused by backflow.

5.3 classical limit of backflow

We would like now to come back to a previous result we have talked about and which require some deeper exloration, namely, the fact that the eigenvalues that allow backflow to happen don't depend on $\hbar$. This is puzzling because if it is really so, then taking the naive classical limit $\hbar \to 0$ wouldn't annihilate the backflow effect, while we know that it is actually a quantum process. There seems to be some apparent problem. Thankfully, we can get some inspiration from some other processes in physics where a similar problem occurs. One of them is the scattering off a step potential, where have also a quantity that does not seem to depend on $\hbar$ and which seems to block us to work efficiently a naive classical limit. In that case, the problem comes from the fact that considering a real step function potential is actually unphysical, and it can be show that it is sufficient to sliglty smoothen it to restore completely the dependence into $\hbar$, allowing us to take a classical limit that annihilates the effect.

The idea here is broadly the same, and we can thus legitimely suspect that there is a quantity that should be (at least) slightly modified to show that eigenvalues are indeed functions of $\hbar$. Following our inspiration from the scattering example we mentioned, let us try to see if defining the flux with quasiprojectors instead of exact projectors as we did, could be helpful. As quasiprojector let us take

$$Q = \int_{0}^{\infty} \mathrm{d}y\, \delta_\sigma(\hat{x} - y) \tag{5.24}$$

where $\delta_\sigma(\hat{x} - y)$ is a smoothed delta-function of the form

$$\delta_\sigma(\hat{x} - y) = \frac{1}{(2\pi\sigma^2)^{1/2}}\, exp(-\frac{(\hat{x} - y)^2}{2\sigma^2}) \tag{5.25}$$

which goes to zero when $\sigma \to 0$, making the quasiprojector beccoming an exact projector.

with this smoothed δ-function, the current operator becomes

$$\hat{J} = \frac{1}{2m}(\hat{p}\delta_\sigma(\hat{x}) + \delta_\sigma(\hat{x})\hat{p}) \tag{5.26}$$

the interesting consequence of this rewriting is that now, the flux contains a new factor, that is exponential, and depending on a certain quantity $a = 2m\sigma^2/\hbar T$

$$F(-T/2, T/2) = \frac{1}{\pi}\int_0^\infty \mathrm{d}u \int_0^\infty \mathrm{d}v\, \phi^*(u)\, \frac{sin(u^2 - v^2)}{u - v} e^{-a^2(u-v)^2} \phi(v) \tag{5.27}$$

and this factor appears also in the eigenvalue equation:

$$\frac{1}{\pi}\int_0^\infty \mathrm{d}v\, \phi^*(u)\, \frac{sin(u^2 - v^2)}{u - v} e^{-a^2(u-v)^2} \phi(v) = \lambda\phi(u) \tag{5.28}$$

this means that the eigenvalue now depends on the parameter a, which itself depends on $\hbar$. So we actually do have a dependence on $\hbar$! This allow us to take the classical limit in the naive sense $\hbar \to 0$. In fact, it is possible to show numerically that the eigenvalues that are solutions of our eigenvalue equation, are bounded from below:

$$\lambda(a) \geq -c_{bm} \tag{5.29}$$

and increase according to the expression

$$\lambda(a) \approx -\frac{1}{a^2} \tag{5.30}$$

In fact, it can be shown numerically under the assumption of the eigenvalues being a function of this parameters a, that the backflow effect goes to zero in the classical limit, while the positive eigenvalue are only little affected. This proves that the apparent independence of the eigenvalues with respect to Planck's constant is only an artificial artefact coming from our mathematical description chosen to model the backflow, and that, with a more accurate model ((namely, involving this parameter a), it is possible to restore a reasonable behavior coherent with what we expect to happen for a behavior that is quantum in its very nature: to disappear in the classical limit.

5.4 backflow and arrival time

In this last section of our work, we would like to say some words about how we can establish a simple connection between backflow and arrival time. The idea we will develop is simple: we will see that arrival time can be used to show if backflow is present or not. We will need to pay attention to the method we decide to model this arrival time. We will use in this section many of the information we have talked about throughout this dissertation. In the simplest case, we just do a measure to see if a particle is present in x<0 at time $t_1 and if it is present at$ x>0$at time$ t_2. The probability will then be

$$p(t_1, t_2) =< \psi|\bar{P}(t_1)P(t_2)\bar{P}(t_1)|\psi > \tag{5.31}$$

which becomes, in terms of the flux operator $\hat{J}$:

$$\begin{aligned} p(t_1, t_2) &=< \psi|\bar{P}(t_1)(P(t_2) - P(t_1))\bar{P}(t_1)|\psi > \\ &= \int_{t_1}^{t_2} \mathrm{d}t \ < \psi|\bar{P}(t_1)\hat{J}(t)\bar{P}(t_1)|\psi > \end{aligned} \tag{5.32}$$

this last equation is positive. In this simple case, backflow will be present if we have a negative flux despite having a positive probability.

Now we can use a more detailed model, using a complex potential, as we did many times previously in this work. We already know that in this case, the arrival time distribution will be

$$\begin{aligned} \Pi(\tau) &= -\frac{dN}{d\tau} \\ &= 2V_0 < \psi|e^{(iH_0 - V_0\theta(\hat{x}))\tau}\theta(\hat{x})e^{(-iH_0 - V_0\theta(\hat{x}))\tau}|\psi > \end{aligned} \tag{5.33}$$

to find the expression that relates $Pi(\tau)$ to $\hat{J}$, we first differentiate with restpect to τ:

$$\frac{d\Pi}{d\tau} = -2V_0\Pi + 2V_0 < \psi|e^{(iH_0 - V_0\theta(\hat{x}))\tau}\hat{J}e^{(-iH_0 - V_0\theta(\hat{x}))\tau}|\psi > \tag{5.34}$$

and then we simply solve the obtained differential equation, which gives us

$$\Pi(\tau) = 2V_0 \int_{-\infty}^{\tau} \mathrm{d}t\, e^{-2V_0(\tau - t)} < \psi|e^{(iH_0 - V_0\theta(\hat{x}))t}\hat{J}e^{(-iH_0 - V_0\theta(\hat{x}))t}|\psi > \tag{5.35}$$

the probability for crossing between $[t_1, t_2]$ will then be

$$p(t_1, t_2) = \int_{t_1}^{t_2} \mathrm{d}t\, \Pi(t) \tag{5.36}$$

let us work in the approximation of small V_0. We then get

$$\Pi(\tau) \approx 2V_0 \int_{-\infty}^{\tau} \mathrm{d}t\, e^{-2V_0(\tau-t)} < \psi_t|\hat{J}|\psi_t > \tag{5.37}$$

The current can be extracted from this last equation by deconvolution, and from there we get the flux, allowing us to deduce the presence of backflow.

Chapter 6

Conclusion

We have finally arrived at the end of our work. It seems now clear that there is some consistency in the various approaches we have covered through this dissertation, in the sens that arrival time appears to be a concept that can be studied with apparently veru different methods, through not necessarily completely disjoint: for example, we have briefly mentioned the fact that there is a deep correspondenc between the path integral approach and the decoherent histories one. this meakes sense since, from a certain point of view, we can say that to a certain history must correspond a certain path. Even though, it is very reassuring to see the consisetnce our the model we have talked about.

Now, they are indeed man problems tha we could have talked about but that we didn't study by lack of time and space, and it should be understood that this dissertation covers only a little drop in the sea of research regarding this topic.

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