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A Path Integral for Classical Dynamics

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Chapter 1

Introduction

In this thesis, we focus on what can be called *quantum-classical divide*, which is one of the main ingredients in order to investigate the relation between the classical and the quantum theories. Although quantum mechanics has been verified with high accuracy in experiments, even today is not clear "how it works" and in particular what this theory is saying about the nature of reality. One way think of quantum mechanics as a list of procedures, specified as a list of instructions of what to do in the lab; this is very important but is not enough to explain, for example, *why* we obtain certain results with certain frequencies, when we do a measurement, or if the wave function is a real entity or not. To fill the gap between the experimental data and our knowledge of reality we need an *interpretation* of quantum mechanics. We learn from history that a better understanding can lead to unexpected new results. For instance, thanks to Bell's studies concerning entanglement, hidden variables, and so on, today enormous steps forward have been done in quantum information theory and towards quantum computation. After a century of quantum mechanics, the debate about the relation between quantum physics and the familiar classical world continues and in this thesis we want to contribute a little to this topic.

We start by reviewing some elementary facts concerning the path integral formalism (see [1, 2, 3, 4, 5]) for the wave function of a non-relativistic spinless particle in one dimension, in order to extend these results for the density matrix. Formally, chosen an initial density matrix, we are able to follow its evolution in time, and in particular, the matrix elements allow us to derive predictions about the interesting physical quantities. Thanks to an idea presented in [6], see also [7], we demonstrate that for Hamiltonian dynamics the Liouville equation differs from the von Neumann equation only by a characteristic *superoperator*. The superoperator is not an ordinary operator that acts on Hilbert space, a crucial difference is found in the interaction between the bra- and ket- states. The related Hilbert space and its dual, therefore, are coupled, unlike the case of quantum mechanics. We introduce the *Liouville space* [8, 9], that is the space where superoperators can be defined.

Employing Liouville space (instead of Hilbert space), we describe time evolution of density matrices in terms of path integrals which are formally identical for quantum and classical mechanics. This allows to import tools developed for Feynman path integrals, in particular, we calculate the Green's functions of the evolution equations. An additional interaction term of a new kind in the relevant action turns out to encode the difference between the classical and the quantum mechanical Green's functions. As a result, we note the equivalence of the Liouville and von Neumann equations for constant, linear, and quadratic potentials, so we are motivated to investigate the difference, for instance, in cases of anharmonic potentials. Therefore, in order to study potentials that cannot be solved exactly, we derive a perturbation theory, in a similar way to derivation for ordinary quantum mechanics [11, 12] . A new type of Feynman diagrams appears . The third chapter is devoted to the calculus of this perturbative expansion and we give an illustration of how it works. Firstly, we calculate exactly, for a massive particle, the free Green's function and apply it to describe the evolution of a classical particle and of a Gaussian density matrix. Secondly, we calculate perturbatively the effect of an anharmonic potential to first order in the coupling constant respectively, for the quantum and the classical mechanics. Choosing an initial density matrix representing a plane wave, we study how it evolves in time for quantum and classical mechanics and we compare graphically these results in order to understand the difference between these two theories.

The last chapter presents the generalization for the case of two particles. The Liouville equation, the path integral, the pertubative expansion, are re-derived. As a results of the parallel study of classical and quantum evolution, we find indications for new aspects of (dynamically assisted) entanglement (generation) [13]. Our findings suggest to distinguish *intra-* from *inter-space entanglement*. The first one is the usual generation of entanglement due to the commutator structure of the evolution operators for quantum mechanics, the second one is due to the particular feature of classical evolution that it couples bra-states with ket-states.

Concerning the quantum-classical divide, the present analysis shows that there is a deep formal similarity between classical and quantum mechanics in a suitable representation as developed here. However, more studies are required. Recently, in the article [14], there is affirmation to replace the usual slogan "Shut up and calculate" by "Shut up and contemplate"; we think that a good synthesis may be *"Take your time, contemplate, and then calculate"*.

Chapter 2

Path integral formalism

2.1 From the Schrödinger equation to the path integral for the propagator

In this chapter, we review some elementary facts about the path integral formalism [1, 2, 3, 4, 5] . We consider the Schrödinger equation for the wavefunction of a nonrelativistic spinless particle in one dimension

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t} \quad , \tag{2.1}$$

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \hat{V} \quad . \tag{2.2}$$

The path integral formalism is helpful to calculate the propagator or Green's function G wich satisfies the equation (in operator notation)

$$\left(\hat{H} - i\hbar\frac{\partial}{\partial t}\right)\hat{G}(t,t_0) = -i\hbar I_d\delta(t-t_0) \quad , \tag{2.3}$$

where I_d denotes the identity matrix. The Green's function is often employed to describe the evolution in time of the wavefunction. Since we are interested in the propagation in space-time, we work in coordinate space. Then, the above equation becomes

$$\left(\hat{H}(x) - i\hbar\frac{\partial}{\partial t}\right)G(x,t;y,t_0) = -i\hbar\delta(x-y)\delta(t-t_0) \quad , \tag{2.4}$$

where $\hat{H}(x)$ is

$$\hat{H}(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \quad , \tag{2.5}$$

and the function G is defined by

$$G(x,t;y,t_0) \equiv \langle x|\hat{G}(t,t_0)|y\rangle \quad . \tag{2.6}$$

For time independent $\hat{H}$, it is straightforward to obtain an operator solution of (2.3)

$$\hat{G}(t,t_0) = \theta(t-t_0)exp\left[-\frac{i\hat{H}(t-t_0)}{\hbar}\right] \quad , \tag{2.7}$$

where θ is the step function. Therefore, for $t > t_0$, in coordinate space we obtain

$$G(x,t;y,t_0) = \langle x|e^{-i\hat{H}(t-t_0)/\hbar}|y\rangle \quad . \tag{2.8}$$

Let $\lambda = i(t-t_0)/\hbar$, we can then write

$$G(x,t;y,t_0) = \langle x|\left(e^{-\lambda(\hat{T}+\hat{V})/N}\right)^N|y\rangle \quad . \tag{2.9}$$

Following this simple trick, we employ the Trotter product formula (see Appendix, [1], [5]), and find for the propagator

$$G(x,t;y,t_0) = \lim_{N\to\infty}\langle x|(e^{-\lambda\hat{T}/N}e^{-\lambda\hat{V}/N})^N|y\rangle \quad . \tag{2.10}$$

Starting from here, is easy to arrive at the path integral. We insert the identity operator

$$\int dx_j|x_j\rangle\langle x_j|, \quad j = 1, ..., N-1 \quad , \tag{2.11}$$

between each term in the product in (2.10), where $|x_j\rangle = |x(t_j)\rangle$ is a complete set of states at time $t_j = t_0 + \frac{j}{N}(t-t_0)$. This gives

$$G(x,t;y,t_0) = \lim_{N\to\infty}\int dx_1\cdots dx_{N-1}\prod_{j=0}^{N-1}\langle x_{j+1}|e^{-\lambda\hat{T}/N}e^{-\lambda\hat{V}/N}|x_j\rangle \quad , \tag{2.12}$$

(for convenience, we have chosen $x_0 = y,\ x_N = x$). In order to calculate the matrix elements in the integral written above, we note that the multiplicative operator $\hat{V}$ is diagonal in coordinate space, so we can immediately write

$$exp(-\frac{\lambda\hat{V}}{N})|x_j\rangle = |x_j\rangle exp(-\frac{\lambda V(x_j)}{N}) \quad . \tag{2.13}$$

For the coordinate space matrix element of $exp(-\lambda\hat{T}/N)$, the situation is a little bit more complicated and, to obtain this, we insert a complete set of momentum states

$$I_d = \int dp\ |p\rangle\langle p| \quad , \qquad \langle p|\xi\rangle = (2\pi\hbar)^{-\frac{1}{2}} exp(-\frac{ip\xi}{\hbar}) \quad . \tag{2.14}$$

This yields

$$\langle\eta|e^{-\lambda\hat{T}/N}|\xi\rangle = \int dp\langle\eta|e^{-\lambda\hat{T}/N}|p\rangle\langle p|\xi\rangle \ = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dp\ e^{-\lambda p^2/2mN} e^{ip(\eta-\xi)/\hbar} \quad . \tag{2.15}$$

We meet here for the first time the omnipresent Gaussian integral

$$\int_{-\infty}^{+\infty} dy\ e^{-ay^2+by} = (\frac{\pi}{a})^{1/2} e^{b^2/4a} \quad . \tag{2.16}$$

Using this, we obtain

$$\langle\eta|e^{-\lambda\hat{T}/N}|\xi\rangle = (\frac{mN}{2\pi\lambda\hbar^2})^{1/2} e^{-mN(\eta-\xi)^2/2\lambda\hbar^2} \quad . \tag{2.17}$$

Inserting this result in the propagator's expression (2.12), we find

$$G(x,t;y,t_0) = \tag{2.18}$$
$$\lim_{N\to\infty}\int dx_1\cdots dx_{N-1}(\frac{mN}{2\pi\lambda\hbar^2})^{N/2}\prod_{j=0}^{N-1} exp\left[-\frac{m(x_{j+1}-x_j)^2 N}{2\lambda\hbar^2} - \frac{\lambda V(x_j)}{N}\right].$$

For a better interpretation of this formula, we introduce $\varepsilon = (t-t_0)/N = \hbar\lambda/iN$, which represents the time interval between the states $|x(t_j)\rangle$. Rearranging the exponentials, we get

$$G(x,t;y,t_0) = \tag{2.19}$$
$$\lim_{N\to\infty}\int dx_1\cdots dx_{N-1}(\frac{m}{2\pi i\hbar\varepsilon})^{N/2} exp\left[\frac{i\varepsilon}{\hbar}\sum_{j=0}^{N-1}\left(\frac{m}{2}(\frac{x_{j+1}-x_j}{\varepsilon})^2 - V(x_j)\right)\right].$$

Equation (2.19) is the path integral expression for the propagator. Considering the limit $\varepsilon \to 0$, we can interpret the sum in the exponential as a Riemann integral

$$\sum_{j=0}^{N-1} \varepsilon \left(\frac{m}{2} (\frac{x_{j+1} - x_j}{\varepsilon})^2 - V(x_j) \right) \sim \int_0^t d\tau \left(\frac{1}{2} m (\frac{dx}{d\tau})^2 - V(x) \right) \quad . \tag{2.20}$$

The integrand here is just the classical Lagrangian, corresponding to the Hamiltonian operator H considered at the beginning of this chapter

$$L = \frac{m}{2} \left(\frac{dx}{d\tau} \right)^2 - V(x) \quad . \tag{2.21}$$

So the integral presents the action

$$S = \int L \; d\tau \quad . \tag{2.22}$$

We can formally re-write (2.19)

$$G(x, t; y, t_0) = \int \mathcal{D}[x(\tau)] e^{\frac{i}{\hbar} S[x]} \quad , \tag{2.23}$$

where we have defined

$$\int \mathcal{D}[x(\tau)] = \lim_{N \to \infty, \varepsilon \to \ 0} \int dx_1 \cdots dx_{N-1} (\frac{m}{2\pi i \hbar \varepsilon})^{N/2} \quad . \tag{2.24}$$

The formula (2.23) is the path integral representation of the Green's function. We can interpret this strange integral as a "sum over all possible paths". In fact, the particle travels from y to x through a series of intermediate steps $x_1, ..., x_{N-1}$, which are separated by a time interval ε. This intermediate steps define a "broken path". When we take the continuum limit $\varepsilon \to 0$ and do the integral, we obtain the interpretation of sum over possible path.

2.2 Evolution of the density matrix

According to the derived path integral representation for the Green's function, now we want to write an evolution equation for the density matrix. In operator notation we can write

$$\hat{\rho}(t) = \hat{G}(t,t_0)\hat{\rho}(t_0)\hat{G}^\dagger(t,t_0) \quad . \tag{2.25}$$

Our interest is to calculate the matrix elements in coordinate space

$$\begin{aligned}\langle x|\hat{\rho}(t)|y\rangle \equiv \rho(x,y;t) &= \int d\eta d\xi \ \langle x|\hat{G}(t,t_0)|\xi\rangle\langle\xi|\hat{\rho}(t)|\eta\rangle\langle\eta|\hat{G}^\dagger(t,t_0)|y\rangle \\ &= \int d\eta d\xi \ G(x,t;\xi,t_0)\rho(\xi,\eta;t_0)G(\eta,t_0;y,t) \quad . \end{aligned} \tag{2.26}$$

We can see that two propagations are present, one for t_0 to t and the other for t to t_0, attributable to the structure of the density matrix. We can call them, respectively, the "forward" and the "backward" propagations. "Forward" is the same as what we have derived in the previous section

$$G(x,t;\xi,0) = \tag{2.27}$$

$$\lim_{N\to\infty,\varepsilon\to 0^+} \int dx_1 \cdots dx_{N-1} (\frac{m}{2\pi i\hbar\varepsilon})^{N/2} exp\left[\frac{i\varepsilon}{\hbar}\sum_{j=0}^{N-1}\left(\frac{m}{2}(\frac{x_{j+1}-x_j}{\varepsilon})^2 - V(x_j)\right)\right],$$

for simplicity we have fixed $t_0 = 0$, and we have considered $x_0 = \xi$, $x_N = x$, $\varepsilon = t/N$. The backward propagation can be expressed as

$$G(\eta,0;y,t) = \tag{2.28}$$

$$\lim_{N\to\infty,\varepsilon'\to 0^-} \int dx'_1 \cdots dx'_{N-1} (\frac{m}{2\pi i\hbar\varepsilon'})^{N/2} exp\left[\frac{i\varepsilon'}{\hbar}\sum_{j=0}^{N-1}\left(\frac{m}{2}(\frac{x'_{j+1}-x'_j}{\varepsilon'})^2 - V(x'_j)\right)\right],$$

where we have considered $t'_j = t + j\varepsilon'$, $\varepsilon' = -t/N$, $x'_j = x'(t'_j)$ with these boundary conditions $x'_N = \eta$, $x'_0 = y$. Taking the respective limits we obtain

$$\lim_{\varepsilon\to 0^+} exp\left[\frac{i\varepsilon}{\hbar}\sum_{j=0}^{N-1}\left(\frac{m}{2}(\frac{x_{j+1}-x_j}{\varepsilon})^2 - V(x_j)\right)\right] = exp\left(\frac{i}{\hbar}\int_0^t L(x(\tau))d\tau\right) \quad , \tag{2.29}$$

$$\lim_{\varepsilon'\to 0^-} exp\left[\frac{i\varepsilon'}{\hbar}\sum_{j=0}^{N-1}\left(\frac{m}{2}(\frac{x'_{j+1}-x'_j}{\varepsilon'})^2 - V(x'_j)\right)\right] = exp\left(\frac{i}{\hbar}\int_t^0 L(x'(\tau'))d\tau'\right) \quad . \tag{2.30}$$

In order to obtain a better understanding, we use one time variable τ. Since $\tau' = t - \tau$, we obtain

$$exp\left(\frac{i}{\hbar}\int_t^0 L(x'(\tau'))d\tau'\right) = exp\left(-\frac{i}{\hbar}\int_0^t L(\tilde{x}(\tau))d\tau\right) \quad , \tag{2.31}$$

where $\tilde{x}(0) = \eta$ and $\tilde{x}(t) = y$. Then we can write

$$G(\eta, 0; y, t) = G^*(y, t; \eta, 0) \quad . \tag{2.32}$$

This simple equation is very important , because it tells us that we may think of the backward path contribution is the complex conjugate of the forward one. This view will permit us to calculate crucial quantities in a straightforward way, and also to have a clear interpretation. Furthermore, we define the quantities

$$\lim_{N\to\infty}\int dx_1 \cdots dx_{N-1} C(N) \equiv \int \mathcal{D}\left[x(\tau)\right] \quad , \tag{2.33}$$

$$\lim_{N\to\infty}\int d\tilde{x}_1 \cdots d\tilde{x}_{N-1} C^*(N) \equiv \int \mathcal{D}\left[\tilde{x}(\tau)\right] \quad . \tag{2.34}$$

Finally, we arrive at the evolution equation for the density matrix in path integral form

$$\rho(x, y; t) = \int d\xi d\eta \mathcal{D}\left[x(\tau)\right] \mathcal{D}\left[\tilde{x}(\tau)\right] e^{\frac{i}{\hbar}S[x]} \rho(\xi, \eta; 0) e^{-\frac{i}{\hbar}S[\tilde{x}]} \quad . \tag{2.35}$$

In order to achieve a similar path integral for classical dynamics, we examine in the next section the evolution equation in phase space for the classical distribution function.

2.3 Liouville equation and von Neumann equation

In this section, we follow Ref. [6], concerning to the reformulation of Hamiltonian dynamics. We set $\hbar = 1$, for simplicity. Let H be the Hamiltonian of a massive particle interacting with a generic potential $V(x)$

$$H(x, p) = \frac{p^2}{2m} + V(x) \quad . \tag{2.36}$$

An ensemble of these objects is described by a distribution function $\rho(x, p, t)$ in phase space, namely by the probability $\rho(x, p, t)dxdp$ to find an element of this ensemble in a neighboord of the point (x, p). This distribution function evolves according to the Liouville equation

$$-\partial_t \rho = \frac{\partial H}{\partial p}\frac{\partial \rho}{\partial x} - \frac{\partial H}{\partial x}\frac{\partial \rho}{\partial p} = (\frac{p}{m}\partial_x - V'(x)\partial_p)\rho \quad . \tag{2.37}$$

In order to build a connection between the matrix elements of the density matrix and the classical distribution function, we replace the momentum p in favour of a coordinate y making use of the following Fourier transform

$$\mathcal{F}(\rho) \equiv \rho(x,y) = \int dp\ e^{ipy}\rho(x,p,t) \quad . \tag{2.38}$$

The effects of this transformation on each term of the Liouville equation are

$$\partial_t \rho \to \partial_t \rho(x,y)\ , \quad p\partial_x \rho \to \mathcal{F}(p\partial_x\rho) = -i\partial_y \partial_x \rho(x,y)\ , \tag{2.39}$$

$$V'(x)\partial_p \rho \to \mathcal{F}(V'(x)\partial_p\rho) = -iV'(x)y\rho(x,y) \quad . \tag{2.40}$$

Indeed, we calculate

$$\mathcal{F}(p\partial_x\rho) = \int dp\ e^{ipy}p\partial_x\rho(x,p,t) = \int -i\partial_y e^{ipy}\partial_x\rho(x,p,t)dp = -i\partial_y\partial_x\rho(x,y) \quad ,$$

$$\begin{aligned}\mathcal{F}(V'(x)\partial_p\rho) &= \int dp\ e^{ipy}V'(x)\partial_p\rho(x,p,t) = V'(x)\int dp\ e^{ipy}\partial_p\rho(x,p,t) = \\ &= V'(x)\left[e^{ipy}\rho(x,p,t)|_{-\infty}^{\infty} - \int dp\ (\partial_p e^{ipy})\rho(x,p,t)\right] = -iV'(x)y\rho(x,y) \quad .\end{aligned}$$

Therefore, the Fourier transform of the Liouville equation becomes

$$-i\partial_t\rho(x,y) = (\frac{\partial_y\partial_x}{m} - V'(x)y)\rho(x,y) \quad . \tag{2.41}$$

With a clever change of variables

$$Q = x + \frac{y}{2},\quad q = x - \frac{y}{2} \quad , \tag{2.42}$$

we rewrite the Liouville equation, considering

$$x = \frac{Q+q}{2} \ , \quad y = Q - q \ ,$$

$$\partial_y \partial_x \rightarrow \frac{1}{2}(\partial^2_{Q^2} - \partial^2_{q^2}) \ ,$$

$$V'(x)y \rightarrow V'\left(\frac{Q+q}{2}\right)(Q-q) \ .$$

Now we can write

$$i\partial_t \rho(Q,q;t) = (-\frac{1}{2m}\partial^2_{Q^2} + \frac{1}{2m}\partial^2_{q^2} + V'(\frac{Q+q}{2})(Q-q)\ )\rho(Q,q;t) \ . \tag{2.43}$$

Furthermore, if we add/subtract by hand the quantity $V(Q) - V(Q) + V(q) - V(q)$, we find

$$i\partial_t \rho(Q,q;t) = (\ \hat{H}(Q) - \hat{H}(q) + \mathcal{E}(Q,q)\ )\rho(Q,q;t) \ , \tag{2.44}$$

where

$$\hat{H}(Q) = -\frac{1}{2m}\partial^2_{Q^2} + V(Q) \ , \tag{2.45}$$

$$\hat{H}(q) = -\frac{1}{2m}\partial^2_{q^2} + V(q) \ , \tag{2.46}$$

$$\mathcal{E}(Q,q) = V(q) - V(Q) + V'(\frac{Q+q}{2})(Q-q) \ . \tag{2.47}$$

In this way, we have constructed a connection between the matrix elements of the density matrix and the classical distribution function. The equation (2.44) can be seen as a matrix element (between states $\langle Q|$ and $|q\rangle$) of the von Neumann equation plus an additional term.

$$i\partial_t \widehat{\rho} = [\widehat{H}, \widehat{\rho}\ ] + \mathcal{E}\widehat{\rho} \ , \tag{2.48}$$

indeed, if we take the matrix element

$$\langle Q|i\partial_t \widehat{\rho}|q\rangle = \langle Q|[\widehat{H}, \widehat{\rho}\ ]|q\rangle + \langle Q|\mathcal{E}\widehat{\rho}|q\rangle \ , \tag{2.49}$$

$$\langle Q|[\widehat{H},\widehat{\rho}\,]|q\rangle = \hat{H}(Q)\rho(Q,q;t) - \rho(Q,q;t)\hat{H}(q) \quad , \tag{2.50}$$

$$\langle Q|\mathcal{E}\widehat{\rho}|q\rangle = \mathcal{E}(Q,q;t)\rho(Q,q;t) \quad . \tag{2.51}$$

By the definition (2.47) of the $\mathcal{E}$, a straightforward calculation shows that for constant, linear, and quadratic potentials this term is equal to zero. Therefore the dynamics of the Liouville equation and of the von Neumann equation are equivalent, in these cases. The $\mathcal{E}$ is not an ordinary operator that acts on Hilbert space, a crucial difference is the interaction between the bra- and ket- states, and to distinguish it from ordinary Hilbert space operators, we call it *superoperator*. The related Hilbert space and its dual, therefore, are coupled, unlike the case of quantum mechanics and we will find this feature also in the path integrals. With the objective to give a home to this superoperator, we introduce in the next section the *Liouville space* or *superspace* [8, 9].

2.4 Liouville space

In this section we give an interpretation of the Liouville equation (2.44) introducing an alternative way of thinking about the density matrix, which makes its evaluation formally identical to the calculation of a wavefunction. We call this *Liouville space* dynamics. We consider the matrix elements ρ_{Qq} of the von Neumann equation

$$\frac{d}{dt}\rho(Q,q;t) = -\frac{i}{\hbar}\int dQ' \left[\hat{H}(Q,Q')\rho(Q',q) - \rho(Q,Q')\hat{H}(Q',q)\right] \quad , \tag{2.52}$$

which can be rearranged in the following form:

$$\frac{d}{dt}\rho(Q,q;t) = -\frac{i}{\hbar}\int dQ'dq' \; \mathcal{H}(Q,q,Q',q')\rho(Q',q';t) \quad , \tag{2.53}$$

where we have defined the so-called Liouville operator $\mathcal{H}$, such that

$$\mathcal{H}(Q,q,Q',q') = \hat{H}(Q,Q')\delta(q'-q) - \hat{H}(q',q)\delta(Q-Q') \quad . \tag{2.54}$$

Considering for the wavefunction an expansion

$$|\psi(t)\rangle = \int dQ \; \psi(Q,t)|Q\rangle \quad , \tag{2.55}$$

with coefficients

$$\frac{d}{dt}\psi(Q,t) = -\frac{i}{\hbar}\int dQ' \; \hat{H}(Q,Q')\psi(Q',t) \quad , \tag{2.56}$$

we can see the analogy between the Schrödinger equation and the von-Neumann equation. The Liouville operator $\mathcal{H}$ has each matrix element labeled by four indices. While in eq. (2.53) it operates on ρ only from the left, we can see from the equivalent eq. (2.52), that it operates from the right *and* from the left. Therefore, we may think of the Liouville operator as a *superoperator*. In *Liouville space* the density matrix is a vector, and the dynamics of the density matrix is more conveniently described in this space. We shall now introduce a few additional definitions, wich will allow us to establish a connection between the time evolution of the wavefunction in ordinary Hilbert space and the evolution of the density operator. It then becomes possible to use all the powerful methods, in particular for our interest in the path integral formalism, developed for the wavefunction.
In Hilbert space, we expand the wavefunction in a complete basis set of vectors $\{|Q\rangle\}$. In this basis $|Q\rangle$ is represented by a unit vector whose Q-th element is 1, and all other elements vanish. Similarly, let us consider the expression

$$\rho = \int dQdq \; \rho(Q,q)|Q\rangle\langle q| \quad , \tag{2.57}$$

$|Q\rangle\langle q|$ is the matrix whose element in the Q-th row and the q-th column is 1 and all other elements vanish.
We may think of the family of operators $|Q\rangle\langle q|$, as a complete set of matrices and rearrange the density operator in the form

$$|\rho\rangle\rangle = \int dQdq \; \rho(Q,q)|Q,q\rangle\rangle \quad , \tag{2.58}$$

where we use a double bracket notation analogous to the brackets used in Hilbert space, and the ket $|Q,q\rangle\rangle$ denotes the Liouville space vector representing the Hilbert space operator $|Q\rangle\langle q|$. We can note the analogy between the equation (2.58) and the following equation

$$|\psi\rangle = \int dQ \; \psi(Q)|Q\rangle \quad . \tag{2.59}$$

We next introduce a bra $\langle\langle Q,q|$ as the Hermitian conjugate to $|Q,q\rangle\rangle$

$$\langle\langle Qq| \equiv (|Qq\rangle\rangle)^\dagger \quad . \tag{2.60}$$

In Liouville space, any Hilbert space operator $\hat{A}$ can be thought of as a vector and be denoted by $|A\rangle\rangle$. This allows us that we can expand it in our basis set

$$A = \int dQdq\ A(Q,q)|Q\rangle\langle q| \quad , \tag{2.61}$$

i.e.

$$|A\rangle\rangle = \int dQdq\ A(Q,q)|Q,q\rangle\rangle \quad . \tag{2.62}$$

We further define a bra vector

$$\langle\langle B| \leftrightarrow B^\dagger \quad , \tag{2.63}$$

and a scalar product of two operators

$$\langle\langle B|A\rangle\rangle \equiv \mathrm{Tr}(B^\dagger A) \quad . \tag{2.64}$$

In particular, we have an orthonormality relation

$$\langle\langle Q,q|Q',q'\rangle\rangle \equiv \mathrm{Tr}\left[|q\rangle\langle Q|Q'\rangle\langle q'|\right] = \delta(Q-Q')\delta(q-q') \quad , \tag{2.65}$$

which is analogous to

$$\langle Q|Q'\rangle = \delta(Q-Q') \quad . \tag{2.66}$$

We can say that the outer products of vectors in Hilbert space constitute the vectors in the higher, Liouville space. Once we accept this, then eq. (2.64) follows naturally: it implies that the scalar product is the trace of the corresponding outer product.
Considering the following scalar product:

$$\langle\langle Q,q|A\rangle\rangle \equiv \mathrm{Tr}\left[|q\rangle\langle Q|A\right] = \int d\tilde{q}\ \langle\tilde{q}|q\rangle\langle Q|A|\tilde{q}\rangle = A(Q,q) \equiv \langle Q|A|q\rangle \quad , \tag{2.67}$$

upon the substitution in (2.62) we have

$$|A\rangle\rangle = \int dQdq|Q,q\rangle\rangle\langle\langle Q,q|A\rangle\rangle, \tag{2.68}$$

which tells us that the completeness condition in Liouville space is

$$\int dQdq\ |Q,q\rangle\rangle\langle\langle Q,q| = 1 \quad . \tag{2.69}$$

This is in analogy with the completeness condition in Hilbert space

$$\int dQ\ |Q\rangle\langle Q| = 1 \quad . \tag{2.70}$$

A collection of objects vectors $|A\rangle\rangle$ together with the operation of addition $|aA+bB\rangle\rangle \equiv aA\rangle\rangle\ + bB\rangle\rangle$, where a and b are complex numbers, and the scalar product form a linear vector space. The *Liouville space* is therefore a linear vector space in which ρ (and any other operator) is a vector.
We can now proceed one step further and introduce an outer product of the Liouville space vectors, which will allow us to define, in general, a superoperator. A superoperator in Liouville space is defined by

$$\mathcal{F} = \int dQdqdQ'dq'\ |Q,q\rangle\rangle\langle\langle Q,q|\mathcal{F}|Q',q'\rangle\rangle\langle\langle Q',q'| \quad , \tag{2.71}$$

with Liouville space matrix elements

$$\mathcal{F}(Q,q,Q',q') \equiv \langle\langle Q,q|\mathcal{F}|Q',q'\rangle\rangle \quad . \tag{2.72}$$

Furthermore, we can define the Hermitian conjugate of a superoperator by its action on the left

$$\mathcal{F}(Q,q,Q',q') \equiv \langle\langle Q,q|\mathcal{F}Q',q'\rangle\rangle = \langle\langle \mathcal{F}^\dagger Q,q|Q',q'\rangle\rangle = \left(\langle\langle\ Q',q'|\mathcal{F}^\dagger Q,q\rangle\rangle\right)^* \quad , \tag{2.73}$$

i.e.

$$\mathcal{F}(Q,q,Q',q')^* = \mathcal{F}^\dagger(Q',q',Q,q) \quad , \tag{2.74}$$

that gives us the condition of self-adjointness

$$\mathcal{F}(Q,q,Q',q')^* = \mathcal{F}(Q',q',Q,q) \quad . \tag{2.75}$$

Finally, we are able to give a well defined interpretation of the Liouville equation (2.44). Indeed if we define a super-Hamiltonian

$$\begin{aligned}\langle\langle Q,q|\mathcal{H}'|Q',q'\rangle\rangle &= (\ \mathcal{H}(Q,q,Q',q') + \mathcal{E}(Q,q,Q',q')\ ) \\ &= \delta(Q-Q')\delta(q-q')(\hat{H}(Q) - \hat{H}(q) + \mathcal{E}(Q,q)) \quad . \end{aligned} \tag{2.76}$$

we can re-write (2.44) as

$$\begin{aligned}\langle\langle Q,q|i\partial_t\rho\rangle\rangle = i\partial_t\rho(Q,q;t) &= \int dQ'dq'\ \mathcal{H}'(Q,q,Q',q')\rho(Q',q';t) \\ &= (\hat{H}(Q) - \hat{H}(q) + \mathcal{E}(Q,q))\rho(Q,q;t) \quad . \end{aligned} \tag{2.77}$$

2.5 Path integral on Liouville space

We want to write a path integral expression for the Green's function of the Liouville equation. A formal solution, in Liouville space, for the Liouville equation is

$$|\rho(t)\rangle\rangle = e^{-i\mathcal{H}'t/\hbar}|\rho(0)\rangle\rangle \quad , \tag{2.78}$$

where $\mathcal{H}' = \mathcal{H} + \mathcal{E}$ is the super-Hamiltonian 2.76. We want to know the matrix element

$$\langle\langle Q,q|\rho(t)\rangle\rangle = \int dQ'dq'\ \langle\langle Q,q|e^{-i\mathcal{H}'t/\hbar}|Q',q'\rangle\rangle\langle\langle Q',q'||\rho(0)\rangle\rangle \quad . \tag{2.79}$$

For our purposes, we can use the Trotter-product formula for superoperators (we will give more detail in the Appendix), since the considered superhamiltonian is self-adjoint. Therefore we obtain

$$e^{-\lambda\mathcal{H}'} = \lim_{N\to\infty}\left(e^{-\frac{\lambda}{N}\mathcal{T}}e^{-\frac{\lambda}{N}\mathcal{V}}\right)^N \quad , \tag{2.80}$$

where $\lambda = it/\hbar$, and

$$\mathcal{T}(Q,q,Q',q') = \delta(Q-Q')\delta(q-q')(-\frac{\hbar^2}{2m}\partial^2_{Q^2} + \frac{\hbar^2}{2m}\partial^2_{q^2}) \tag{2.81}$$

$$\mathcal{V}(Q,q,Q',q') = \delta(Q-Q')\delta(q-q')(V(Q) - V(q)) \quad \text{for} \quad \mathcal{E} = 0 \tag{2.82}$$

$$\mathcal{V}(Q,q,Q',q') = \delta(Q-Q')\delta(q-q')\Big((Q-q)V'(\frac{Q+q}{2})\Big) \quad \text{for} \quad \mathcal{E} \neq 0 \tag{2.83}$$

Again we can see the benefits of the Liouville space dynamics, we are able to achieve two different path integrals in one treatment. The first for the propagator of the von Neumann equation, i.e. $\mathcal{E} = 0$, and the second for the Liouville equation, i.e. $\mathcal{E} \neq 0$.
Now we are ready to calculate the superpropagator

$$\mathcal{G}(Q, q, t; Q', q', 0) = \langle\langle Q, q| e^{-\lambda \mathcal{H}'} |Q', q'\rangle\rangle = \lim_{N\to\infty} \langle\langle Q, q| (e^{-\frac{\lambda}{N}\mathcal{T}} e^{-\frac{\lambda}{N}\mathcal{V}})^N |Q', q'\rangle\rangle \quad . \tag{2.84}$$

Like in the previous section, we insert a complete set of superstates

$$\int dQ_j dq_j \; |Q_j, q_j\rangle\rangle\langle\langle Q_j, q_j| = I \qquad j = 1, ..., N-1 \quad , \tag{2.85}$$

which yields

$$\mathcal{G}(Q, q, t; Q', q', 0) = \tag{2.86}$$
$$\lim_{N\to\infty} \int (dQ_1 dq_1) \cdots (dQ_{N-1} dq_{N-1}) \prod_{j=0}^{N-1} \langle\langle Q_{j+1}, q_{j+1}| e^{-\frac{\lambda}{N}\mathcal{T}} e^{-\frac{\lambda}{N}\mathcal{V}} |Q_j, q_j\rangle\rangle \quad .$$

The superoperator $\mathcal{V}$ is diagonal in coordinate space reppresentation

$$e^{-\frac{\lambda}{N}\mathcal{V}} |Q_j, q_j\rangle\rangle = |Q_j, q_j\rangle\rangle e^{-\frac{\lambda}{N}\mathcal{V}(Q_j, q_j)} \quad . \tag{2.87}$$

Next we need coordinate space matrix element of $e^{-\frac{\lambda}{N}\mathcal{T}}$. For this, we use a complete set of momentum superstates

$$\langle\langle P_\xi, P_\eta| = \frac{1}{2\pi\hbar} \int d\xi d\eta \; e^{-iP_\xi \xi} e^{+iP_\eta \eta} \langle\langle \xi, \eta| \quad , \tag{2.88}$$

such that

$$\langle\langle P_\xi, P_\eta | Q, q\rangle\rangle = \frac{1}{2\pi\hbar} e^{-\frac{i}{\hbar} P_\xi Q} e^{+\frac{i}{\hbar} P_\eta q} \quad , \tag{2.89}$$

$$\langle\langle Q_{j+1}, q_{j+1}| e^{-\frac{\lambda}{N}\mathcal{T}} |Q_j, q_j\rangle\rangle = \int dP_\xi dP_\eta \; \langle\langle Q_{j+1}, q_{j+1}| e^{-\frac{\lambda}{N}\mathcal{T}} |P_\xi, P_\eta\rangle\rangle \langle\langle P_\xi, P_\eta | Q_j, q_j\rangle\rangle \quad . \tag{2.90}$$

Now we can write

$$e^{-\frac{\lambda}{N}\mathcal{T}}|P_\xi, P_\eta\rangle\rangle = |P_\xi, P_\eta\rangle\rangle e^{-\frac{\lambda}{N}\mathcal{T}(P_\xi,P_\eta)} \quad , \tag{2.91}$$

thus we obtain

$$\int dP_\xi dP_\eta \ e^{-\frac{\lambda}{N}\mathcal{T}(P_\xi,P_\eta)}\langle\langle Q_{j+1}, q_{j+1}|P_\xi, P_\eta\rangle\rangle\langle\langle P_\xi, P_\eta|Q_j, q_j\rangle\rangle \quad ,$$

$$\int \frac{dP_\xi dP_\eta}{(2\pi\hbar)^2} \ e^{-\frac{\lambda}{N}\mathcal{T}(P_\xi,P_\eta)} e^{\frac{i}{\hbar}P_\xi(Q_{j+1}-Q_j)} e^{\frac{i}{\hbar}P_\eta(q_j-q_{j+1})} \quad , \tag{2.92}$$

where

$$e^{-\frac{\lambda}{N}\mathcal{T}(P_\xi,P_\eta)} = e^{-\frac{\lambda}{N}(\frac{P_\xi^2}{2m}-\frac{P_\eta^2}{2m})} \quad . \tag{2.93}$$

Therefore, we encounter the following two Gaussian integrals that know the solution

$$\int \frac{dP_\xi}{(2\pi\hbar)} e^{-\frac{\lambda}{N}\frac{P_\xi^2}{2m}} e^{\frac{i}{\hbar}P_\xi(Q_{j+1}-Q_j)} = \frac{1}{(2\pi\hbar)}(\frac{2\pi m N}{\lambda})^{\frac{1}{2}} e^{-\frac{mN(Q_{j+1}-Q_j)^2}{2\lambda\hbar^2}} \quad , \tag{2.94}$$

$$\int \frac{dP_\eta}{(2\pi\hbar)} e^{\frac{\lambda}{N}\frac{P_\eta^2}{2m}} e^{\frac{i}{\hbar}P_\eta(q_j-q_{j+1})} = \frac{1}{(2\pi\hbar)}(\frac{2\pi m N}{-\lambda})^{\frac{1}{2}} e^{\frac{mN(q_j-q_{j+1})^2}{2\lambda\hbar^2}} \quad . \tag{2.95}$$

Let $\epsilon = \frac{t}{N} = \frac{\hbar\lambda}{iN}$, then $\frac{1}{(2\pi\hbar)}(\frac{2\pi m N}{\lambda})^{\frac{1}{2}} = (\frac{m}{2\pi\hbar i\epsilon})^{\frac{1}{2}}$. Finally, we obtain for the superpropagator

$$\begin{aligned} \mathcal{G}(Q,q,t;Q',q',0) &= \lim_{N\to\infty}\int (dQ_1 dq_1)\cdots(dQ_{N-1}dq_{N-1})(\frac{m}{2\pi\hbar i\epsilon})^{\frac{N}{2}}(\frac{m}{2\pi\hbar(-i\epsilon)})^{\frac{N}{2}} \\ &\times \ exp\left[\frac{i\epsilon}{\hbar}\sum_{j=0}^{N-1}\frac{m}{2}\left((\frac{Q_{j+1}-Q_j}{\epsilon})^2-(\frac{q_{j+1}-q_j}{\epsilon})^2\right)-\mathcal{V}(Q_j,q_j)\right] \quad . \end{aligned} \tag{2.96}$$

In the limit $\epsilon \to 0$, the sum in the exponential can be interpreted as a Riemann integral over the path:

$$\sum_{j=0}^{N-1}\frac{m}{2}\left((\frac{Q_{j+1}-Q_j}{\epsilon})^2-(\frac{q_{j+1}-q_j}{\epsilon})^2\right)-\mathcal{V}(Q_j,q_j) \sim \int d\tau\left(\frac{m}{2}(\frac{dQ}{d\tau})^2-\frac{m}{2}(\frac{dq}{d\tau})^2-\mathcal{V}(Q,q)\right) \quad . \tag{2.97}$$

Furthermore, if we define, as in the previous section

$$\lim_{N\to\infty}\int(d\overrightarrow{Q}_1)\cdots(d\overrightarrow{Q}_{N-1})C(N)=\int\mathcal{D}[\overrightarrow{Q}(\tau)] \quad , \tag{2.98}$$

where $\overrightarrow{Q}_i=(Q_i,q_i)$ and $\overrightarrow{Q}(\tau)=(Q(\tau),q(\tau))$, we obtain the expression for the superpropagator

$$\mathcal{G}(\overrightarrow{Q},t;\overrightarrow{Q}',0)=\int\mathcal{D}[\overrightarrow{Q}(\tau)]e^{\frac{i}{\hbar}\mathcal{S}[\overrightarrow{Q}]} \quad . \tag{2.99}$$

This integral has the boundary conditions $\overrightarrow{Q}(t)=\overrightarrow{Q},\ \overrightarrow{Q}(0)=\overrightarrow{Q}'$, and $\mathcal{S}$ is the superaction:

$$\mathcal{S}=\int d\tau\ (\mathcal{T}-\mathcal{V})=\int d\tau\ \mathcal{L} \quad . \tag{2.100}$$

Finally, we arrive at the following evolution equation for the density matrix in the Liouville space formulation

$$\langle\langle Q,q|\rho(t)\rangle\rangle=\rho(Q,q;t)=\int dQ'dq'\int\mathcal{D}[\overrightarrow{Q}(\tau)]e^{\frac{i}{\hbar}\mathcal{S}[\overrightarrow{Q}]}\langle\langle Q',q'|\rho(0)\rangle\rangle \quad . \tag{2.101}$$

2.6 Comparison of Hilbert space and Liouville space path integrals

We want to check that for $\mathcal{E}=0$ the Eqs. (2.35) - (2.101) are equivalent . We begin with rewriting the von Neumann equation

$$i\partial_t\rho(Q,q;t)=(\ \hat{H}(Q)-\hat{H}(q)\ )\rho(Q,q;t) \quad , \tag{2.102}$$

that has the formal solution

$$\hat{\rho}(t)=e^{-it\hat{H}/\hbar}\hat{\rho}(t_0)e^{it\hat{H}/\hbar} \quad . \tag{2.103}$$

Therefore, as in Sec. 2.2, we can rewrite (in terms of the appropriate coordinates Q,q) the eq. (2.35)

$$\rho(Q,q;t)=\int dQ'dq'\int\mathcal{D}[Q(\tau)]\,\mathcal{D}[q(\tau)]\ e^{\frac{i}{\hbar}S[Q]}\rho(Q',q';0)e^{-\frac{i}{\hbar}S[q]} \quad , \tag{2.104}$$

where

$$S\left[Q\right] = \int d\tau \left[\frac{m}{2}(\frac{dQ}{d\tau})^2 - V(Q)\right] \ , \ \ S\left[q\right] = \int d\tau \left[\frac{m}{2}(\frac{dq}{d\tau})^2 - V(q)\right] \ . \tag{2.105}$$

The actions are functionals, and we can multiplicate the two exponential to yield

$$\rho(Q,q;t) = \tag{2.106}$$
$$\int dQ'dq' \int \mathcal{D}\left[Q(\tau)\right]\mathcal{D}\left[q(\tau)\right] e^{\frac{i}{\hbar}\int d\tau\left[\frac{m}{2}(\frac{dQ}{d\tau})^2 - \frac{m}{2}(\frac{dq}{d\tau})^2 - V(Q) + V(q)\right]}\rho(Q',q';0) \ ,$$

which is just the eq. (2.101) with a *separable superaction*

$$\mathcal{S}[Q,q] = S[Q] - S[q] \ . \tag{2.107}$$

We learn that the path integral for quantum mechanics has the particularity that we can separate the phases, because the relevant superaction is separable. This is a consequence of what we noted previously at the end of Sec.2.3, that is the Hilbert space and its dual are uncoupled. Or we may say that the forward path and the backward path are *independent*. For the case $\mathcal{E} \neq 0$, we do not have a separable superaction,

$$\mathcal{S}[Q,q] = S_0[Q] - S_0[q] + S_{int}[Q,q] \ . \tag{2.108}$$

where we have distinguished the free separablesuperaction, that comes from the kinetic term of the action, from the the interacting *nonseparable superaction*, that comes out from the generally *nonseparable superpotential*

$$\mathcal{V}(Q,q) = (Q-q)V'\Big(\frac{Q+q}{2}\Big) \ . \tag{2.109}$$

This feature is characteristic of the Liouville equation, it couples the Hilbert space with its dual, so in this case we may say that the forward path and the backward path influence each other.

Chapter 3

Free particle and perturbative expansion

3.1 Explicit calculus for the superpropagator

In this section, we calculate the free superpropagator (Green's function in Liouville space)

$$\mathcal{G}(Q,q,t;Q',q',0) = \lim_{N\to\infty}\int (dQ_1 dq_1)\cdots(dQ_N dq_N)\ (\frac{m}{2\pi\hbar i\epsilon})^{\frac{N+1}{2}}(\frac{m}{2\pi\hbar(-i\epsilon)})^{\frac{N+1}{2}}\times$$
$$exp\left[\frac{i\epsilon}{\hbar}\sum_{j=0}^{N}\frac{m}{2}\left((\frac{Q_{j+1}-Q_j}{\epsilon})^2-(\frac{q_{j+1}-q_j}{\epsilon})^2\right)\right] \quad , \tag{3.1}$$

where $Q_{N+1}=Q$, $Q_0=Q'$, $q_{N+1}=q$, $q_0=q'$, and $\epsilon=t/(N+1)$. We know the result (see [1], for a detailed calculation for quadratic Lagrangians) for the free propagator, that is

$$G(Q,t;Q',0) = (\frac{m}{2\pi i\hbar t})^{\frac{1}{2}}exp\left[\frac{im}{2\hbar t}(Q-Q')^2\right] \quad . \tag{3.2}$$

We observe that for a free particle the classical path from $(Q',0)$ to (Q,t) is

$$Q(\tau) = Q' + \frac{\tau}{t}(Q-Q') \quad , \tag{3.3}$$

and the classical action is

$$S_c = \int_0^t \frac{m}{2}(\frac{Q-Q'}{t})^2 d\tau \ = \frac{m}{2}\frac{(Q-Q')^2}{t} \quad , \tag{3.4}$$

which is sufficient to obtain the exact propagator for a free particle. Since we can separate the integral over the Q from q (in the case $\mathcal{E}=0$), our aim is to evaluate

$$G^*(q,t;q',0) = \tag{3.5}$$
$$\lim_{N\to\infty}\int dq_1\cdots dq_N\left(\frac{m}{2\pi\hbar(-i\epsilon)}\right)^{\frac{N+1}{2}} exp\left[\frac{-i\epsilon}{\hbar}\sum_{j=0}^{N}\frac{m}{2}\left(\frac{q_{j+1}-q_j}{\epsilon}\right)^2\right] .$$

Here we employ our earlier interpretation that the backward path corresponds to the forward path with a complex conjugated (see eq. (2.32)), contribution to the phase. Let the classical path be

$$q(\tau) = q' + \frac{\tau}{t}(q-q') \quad , \tag{3.6}$$

and the classical action

$$S_c = \int_0^t \frac{m}{2}\left(\frac{q-q'}{t}\right)^2 d\tau \;=\; \frac{m}{2}\frac{(q-q')^2}{t} \quad , \tag{3.7}$$

therefore, we obtain

$$G^*(q,t;q',0) = \left(\frac{m}{2\pi\hbar(-it)}\right)^{\frac{1}{2}} exp\left[\frac{-im}{2\hbar t}(q-q')^2\right] \quad . \tag{3.8}$$

Finally, we find the result for the superpropagator is

$$\begin{aligned} \mathcal{G}(Q,q,t;Q',q',0) &= G(Q,t;Q',0)G^*(q,t;q',0) \\ &= \left(\frac{m}{2\pi\hbar t}\right) exp\left[\frac{im}{2\hbar t}((Q-Q')^2-(q-q')^2)\right] \quad , \end{aligned} \tag{3.9}$$

which is *separable*; the forward path variables Q, Q' are independent of the backward path variables q, q'. We remark that this behaviour reflects the separable action, i.e. the uncoupled Hilbert space and its dual.

3.2 Evolution of a classical particle state

Next, we study the evolution for a classical particle, represented by a point in phase space, in the free case. Let ρ be the distribution function at time $t_0 = 0$

$$\rho(x,p,0) = \delta(x-x_0)\delta(p-p_0) \quad , \tag{3.10}$$

where x_0, p_0 denote, respectively, the initial position and momentum. Firstly, we fix for simplicity $x_0 = 0$. Secondly, we change the variables $(x,p) \Rightarrow (x,y) \Rightarrow (Q,q)$, in order to study the evolution through the known propagator. Finally, we come back to (x,p) to have a physical interpretation in phase space of what happened. The first change gives

$$\rho(x,y;0) = \delta(x) \int dp \; e^{ipy} \delta(p - p_0) = \delta(x) e^{ip_0 y} \quad , \tag{3.11}$$

then

$$\rho(Q',q';0) = \delta\Big(\frac{Q'+q'}{2}\Big) e^{ip_0(Q'-q')} \quad . \tag{3.12}$$

At this point, we are able to calculate the density matrix at a time t,

$$\begin{aligned}
\rho(Q,q;t) &= \int dQ'dq' \; \mathcal{G}(Q,q,t;Q',q',0)\rho(Q',q';0) \\
&= \Big(\frac{m}{2\pi t}\Big) \int dQ' \; e^{\frac{im}{2t}(Q-Q')^2 + ip_0 Q'} \int dq' \; e^{\frac{-im}{2t}(q-q')^2 - ip_0 q'} \delta\Big(\frac{Q'+q'}{2}\Big) \\
&= 2\Big(\frac{m}{2\pi t}\Big) e^{\frac{im}{2t}(Q^2-q^2)} \int dQ' \; e^{\frac{-2im}{t}Q'(\frac{Q+q}{2} - p_0\frac{t}{m})} \\
&= e^{\frac{im}{t}(Q-q)(\frac{Q+q}{2})} \delta\Big(\frac{Q+q}{2} - p_0\frac{t}{m}\Big) \quad .
\end{aligned} \tag{3.13}$$

Now we change back the variables $(Q,q) \Rightarrow (x,y)$

$$\rho(x,y;t) = e^{\frac{im}{t}xy} \delta\Big(x - p_0\frac{t}{m}\Big) \quad , \tag{3.14}$$

and $(x,y) \Rightarrow (x,p)$, which yields

$$\rho(x,p;t) = \delta\Big(x - p_0\frac{t}{m}\Big) \int \frac{dy}{2\pi} e^{\frac{im}{t}xy} e^{-ipy} = \delta\Big(x - p_0\frac{t}{m}\Big) \delta\Big(p - \frac{m}{t}x\Big) \quad . \tag{3.15}$$

Thus, we find the expected result, that is

$$\rho(x,p;t) = \delta\Big(x - p_0\frac{t}{m}\Big) \delta\Big(p - p_0\Big) \quad . \tag{3.16}$$

We learn that the von Neumann equation, which is a typical quantum mechanical equation, also describes the propagation of a free classical particle. This confirms our analysis that Liouville and von Neumann equation coincide for constant, linear, and harmonic potentials.

3.3 Evolution of a Gaussian density matrix

We compare the evolution of a density matrix, which initially represented by a Gaussians wavepackets, in Hilbert and Liouville spaces in the case of free propagation. The evolution of the density matrix with the Liouville space formalism is described by the following equation

$$\rho(Q,q;t) = \int dQ'dq' \int \mathcal{D}\left[Q(\tau)\right]\mathcal{D}\left[q(\tau)\right]\ e^{\frac{i}{\hbar}S[Q]}\rho(Q',q';0)e^{-\frac{i}{\hbar}S[q]}. \tag{3.17}$$

We choose for the initial density matrix

$$\rho(Q',q';0) = Ce^{-\alpha(Q'^2+\ q'^2)}. \tag{3.18}$$

Then we must to calculate

$$\rho(Q,q;t) = C\left(\frac{m}{2\pi\hbar t}\right)\int dQ'dq'\ e^{-\alpha(Q'^2+\ q'^2)}e^{\left[\frac{im}{2\hbar t}((Q-Q')^2-(q-q')^2)\right]}\quad . \tag{3.19}$$

Since we can separate the two integrals, what we really have to know is the solution of only one integral, since both have the same structure:

$$\int dQ' e^{\frac{im}{2\hbar t}(Q-Q')^2}e^{-\alpha Q'^2}\quad . \tag{3.20}$$

We obtain:

$$e^{\beta Q^2}\int dQ' e^{-(\alpha-\beta)Q'^2}e^{-2\beta QQ'} = \left(\frac{\pi}{\alpha-\beta}\right)^{\frac{1}{2}} e^{\frac{\alpha\beta}{\alpha-\beta}Q^2}\quad , \tag{3.21}$$

where $\beta = \frac{im}{2\hbar t}$. The integral for the second, remaining variable q', is of the form

$$\int dq'\ e^{\beta^*(q-q')^2}e^{-\alpha q'^2} = \left(\frac{\pi}{\alpha-\beta^*}\right)^{\frac{1}{2}} e^{\frac{\alpha\beta^*}{\alpha-\beta^*}q^2}\quad . \tag{3.22}$$

At this point, we can write the density matrix at time t

$$\rho(Q,q;t) = \frac{C|\beta|}{(\alpha^2-\beta^2)^{\frac{1}{2}}} e^{\alpha\beta(\frac{Q^2}{\alpha-\beta}-\frac{q^2}{\alpha+\beta})}. \tag{3.23}$$

Now we show that the same result is given by the ordinary Hilbert space formalism. Indeed, we may just consider the following evolution for a Gaussian wave function

$$\psi(Q,t) = \int dQ' \int \mathcal{D}[Q]\ e^{\frac{i}{\hbar}S[Q]}\ \psi(Q',0) \quad , \tag{3.24}$$

where

$$\psi(Q',0) = \sqrt{C} e^{-\alpha Q'^2} \quad . \tag{3.25}$$

Therefore, in order to find the evolution of the wave function, we must to calculate the integral

$$\psi(Q,t) = \sqrt{C}\left(\frac{m}{2\pi\hbar i t}\right)^{\frac{1}{2}} \int dQ'\ e^{\frac{im}{2\hbar t}(Q-Q')^2} e^{-\alpha Q'^2} \quad , \tag{3.26}$$

which is the same integral as in equation (3.20) (except for an overall constant). For the complex conjugate wave function, we obtain:

$$\psi^*(q,t) = \int dq' \int \mathcal{D}[q]\ e^{-\frac{i}{\hbar}S[q]}\ \psi^*(q',0) \quad , \tag{3.27}$$

where

$$\psi^*(q',0) = \sqrt{C} e^{-\alpha q'^2} \quad . \tag{3.28}$$

As above, we must calculate the following integral

$$\psi^*(q,t) = \sqrt{C}\left(\frac{m}{2\pi\hbar(-it)}\right)^{\frac{1}{2}} \int dq' e^{-\frac{im}{2\hbar t}(q-q')^2} e^{-\alpha q'^2} \quad , \tag{3.29}$$

which is the same integral as in equation (3.22) (except for the constant out of the integral). Recalling that we have a pure state, we obtain the final result:

$$\rho(Q,q;t) = \psi(Q,t)\psi^*(q,t) = \frac{C|\beta|}{(\alpha^2-\beta^2)^{\frac{1}{2}}} e^{\alpha\beta(\frac{Q^2}{\alpha-\beta}-\frac{q^2}{\alpha+\beta})}. \tag{3.30}$$

All that we have done in this section can also be repeated for a particle undergoes in constant, linear or quadratic potential. Indeed, in this case, the Liouville and von Neumann equations coincide and classical and quantum mechanics give the same predictions. In the next section, we will develop a perturbative expansion with the aim of calculating the propagators for potentials that cannot be solved exactly– for example, the anharmonic oscillator– and to compare the results respectively obtained from classical and quantum mechanics.

3.4 Perturbative expansion

The following perturbative expansion is an extension of the pertubation theory for ordinary Hilbert space [1, 11, 12]. Now that we know how the density matrix evolves with the free super-Hamiltonian, the next step is to understand how it evolves for a generic superpotential. Consider the superpropagator

$$\mathcal{G}(\overrightarrow{Q},t;\overrightarrow{Q}',0)=\int\mathcal{D}[\overrightarrow{Q}]\ e^{\frac{i}{\hbar}\int_0^t\mathcal{T}(\dot{Q},\dot{q})d\tau}\ e^{-\frac{i}{\hbar}\int_0^t\mathcal{V}(Q,q)d\tau}\quad . \tag{3.31}$$

In general, the last term that describes the interaction is difficult to treat. For this reason, we expand it in a power series

$$exp\left(-\frac{i}{\hbar}\int_0^t\mathcal{V}(Q,q)d\tau\right)=\sum_{j=0}^{\infty}\frac{1}{j!}\left(\frac{-i}{\hbar}\right)^j\left(\int_0^t\mathcal{V}(Q,q)d\tau\right)^j\quad . \tag{3.32}$$

At this point, we can define

$$\mathcal{V}(Q(\tau),q(\tau))=F(\tau)\quad , \tag{3.33}$$

and derive a formula [1] for the N-th power of the integral in the expansion of the exponential of the superpotential, namely

$$\left(\int_0^t\mathcal{V}(Q,q)d\tau\right)^N= \tag{3.34}$$

$$N!\int_0^t d\tau_1\cdots\int_0^{\tau_{N-1}}d\tau_N\ \mathcal{V}(Q(\tau_1),q(\tau_1))\mathcal{V}(Q(\tau_2),q(\tau_2))\cdots\mathcal{V}(Q(\tau_N),q(\tau_N)).$$

We need to analize terms of this kind

$$\mathcal{G}_k(\overrightarrow{Q},t;\overrightarrow{Q}',0)\equiv\frac{1}{k!}\int\mathcal{D}[\overrightarrow{Q}]\ e^{\frac{i}{\hbar}\int_0^t\mathcal{T}(\dot{Q},\dot{q})d\tau}\left(\int_0^t\mathcal{V}(Q,q)d\tau\right)^k\quad . \tag{3.35}$$

The $k = 0$ term is just the free superpropagator already calculated in the previous section, so we consider the $k = 1$ term

$$\mathcal{G}_1(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0) = \int \mathcal{D}[\overrightarrow{Q}] \; e^{\frac{i}{\hbar}\int_0^t \mathcal{T}(\dot{Q},\dot{q})d\tau} \left(\int_0^t \mathcal{V}(Q,q)d\tau \right) \quad , \tag{3.36}$$

i.e.,

$$\begin{aligned} \mathcal{G}_1(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0) &= \sum_{j=0}^{N} \epsilon \int \prod_{i=1}^{N} dQ_i dq_i \; (\frac{m}{2\pi\hbar i\epsilon})^{\frac{N+1}{2}} (\frac{m}{2\pi\hbar(-i\epsilon)})^{\frac{N+1}{2}} \\ &\times \; exp\left[\frac{i\epsilon}{\hbar} \sum_{k=0}^{N} \frac{m}{2} \left[(\frac{Q_{j+1}-Q_j}{\epsilon})^2 - (\frac{q_{j+1}-q_j}{\epsilon})^2 \right] \right] \mathcal{V}(Q_j, q_j) \quad . \end{aligned} \tag{3.37}$$

The integrals over $k = 0, ..., j-1$ and $k = j+1, ..., N$ give just free superpropagators. Then, doing the continuum limit, we obtain

$$\begin{aligned} \mathcal{G}_1(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0) &= \int_0^t d\tau \int d\eta d\xi \; G_0(Q,t;\xi,\tau) G_0^*(q,t;\eta,\tau) \mathcal{V}(\xi,\eta) G_0(\xi,\tau;Q',0) G_0^*(\eta,\tau;q',0) \\ &= \int_0^t d\tau \int d\overrightarrow{\zeta} \, \mathcal{G}_0(\overrightarrow{Q}, t; \overrightarrow{\zeta}, \tau) \mathcal{V}(\overrightarrow{\zeta}) \mathcal{G}_0(\overrightarrow{\zeta}, \tau; \overrightarrow{Q'}, 0) \quad , \end{aligned} \tag{3.38}$$

where we have defined $\overrightarrow{\zeta} = (\xi, \eta)$. Now we consider the case $k = 2$:

$$\mathcal{G}_2(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0) = \frac{1}{2} \int \mathcal{D}[\overrightarrow{Q}] \; e^{\frac{i}{\hbar}\int_0^t \mathcal{T}(\dot{Q},\dot{q})d\tau} \left(\int_0^t \mathcal{V}(Q,q)d\tau \right)^2 \quad . \tag{3.39}$$

Thanks to the formula written above, eq.(3.34), we can evaluate the second power of the potential integral

$$\left(\int_0^t \mathcal{V}(Q,q)d\tau \right)^2 = 2 \int_0^t d\tau \int_0^\tau d\sigma \; \mathcal{V}(Q(\sigma), q(\sigma)) \mathcal{V}(Q(\tau), q(\tau)) \quad . \tag{3.40}$$

Then, using eq.(3.38), we arrive at a recursive formula for the $k = 2$ contribution to the superpropagator, i.e.

$$\begin{aligned} &\mathcal{G}_2(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0) = \\ &\int_0^t d\tau \int_0^\tau d\sigma \int d\overrightarrow{\zeta'} \int d\overrightarrow{\zeta} \, \mathcal{G}_0(\overrightarrow{Q}, t; \overrightarrow{\zeta'}, \tau) \mathcal{V}(\overrightarrow{\zeta'}) \mathcal{G}_0(\overrightarrow{\zeta'}, \tau; \overrightarrow{\zeta}, \sigma) \mathcal{V}(\overrightarrow{\zeta}) \mathcal{G}_0(\overrightarrow{\zeta}, \sigma; \overrightarrow{Q'}, 0) \; , \end{aligned} \tag{3.41}$$

namely

$$\mathcal{G}_2(\overrightarrow{Q},t;\overrightarrow{Q'},0) = \int_0^t d\tau \int d\overrightarrow{\zeta'}\ \mathcal{G}_0(\overrightarrow{Q},t;\overrightarrow{\zeta'},\tau)\mathcal{V}(\overrightarrow{\zeta'})\mathcal{G}_1(\overrightarrow{\zeta'},\tau;\overrightarrow{Q'},0) \quad , \tag{3.42}$$

where we have defined $\overrightarrow{\zeta'} = (\xi', \eta')$. We can generalize, for an arbitrary k, this recursive formula

$$\mathcal{G}_k(\overrightarrow{Q},t;\overrightarrow{Q'},0) = \int_0^t d\tau \int d\overrightarrow{\zeta}\ \mathcal{G}_0(\overrightarrow{Q},t;\overrightarrow{\zeta},\tau)\mathcal{V}(\overrightarrow{\zeta})\mathcal{G}_{k-1}(\overrightarrow{\zeta},\tau;\overrightarrow{Q'},0) \quad . \tag{3.43}$$

Using this result, we can immediately establish that

$$\mathcal{G}(\overrightarrow{Q},t;\overrightarrow{Q'},0) = \mathcal{G}_0(\overrightarrow{Q},t;\overrightarrow{Q'},0) - \frac{i}{\hbar}\int_0^t d\tau \int d\overrightarrow{\zeta}\ \mathcal{G}_0(\overrightarrow{Q},t;\overrightarrow{\zeta},\tau)\mathcal{V}(\overrightarrow{\zeta})\mathcal{G}(\overrightarrow{\zeta},\tau;\overrightarrow{Q'},0) \quad , \tag{3.44}$$

which presents the resummation of the pertubation series in a *Dyson integral equation* for the full superpropagator.

We may give an interpretetion of the individual terms in the expansion

$$\mathcal{G}(\overrightarrow{Q},t;\overrightarrow{Q'},0) = \sum_{j=0}^{\infty}\left(\frac{-i}{\hbar}\right)^j \mathcal{G}_j(\overrightarrow{Q},t;\overrightarrow{Q'},0) \quad . \tag{3.45}$$

We may think of the total sum as the total amplitude for the particle to go from $(\overrightarrow{Q'},0)$ to $(\overrightarrow{Q},t)$. The individual terms in the expansion describe a particular propagation. The first term, i.e. the zeroth order correction in the perturbative expansion, is just the free path between the initial and final points. The Fig.3.1 represents in a Feynman diagram the contribution of first order perturbation theory. Initially, the particle propagates freely from $(Q', q', 0)$ to (ξ, η, τ), then it is subject to the superpotential $\mathcal{V}(\xi, \eta)$, and finally goes again freely from (ξ, η, τ) to (Q, q, t). Furthermore, the integral over space-time, present in the correction itself, represents the various ways of making this path. The higher order corrections have similar interpretations.

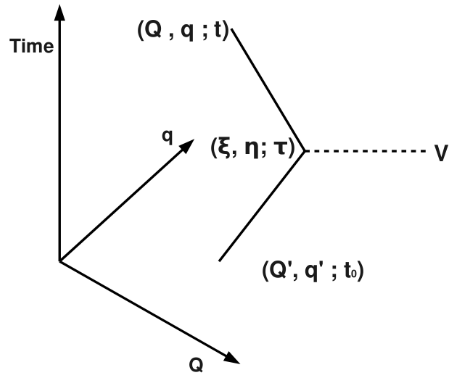

Figure 3.1: Feynman graph for first order perturbation theory.

3.5 First application: the anharmonic oscillator

We want to calculate the first order correction to the propagator in the case of an anharmonic superpotential and also to compare the results obtained from classical and quantum mechanics.

3.5.1 Quantum mechanics

Consider the equation

$$\mathcal{G}_1(\overrightarrow{Q},t;\overrightarrow{Q'},0)=\int_0^t d\tau\int d\eta d\xi\; G_0(Q,t;\xi,\tau)G_0^*(q,t;\eta,\tau)\mathcal{V}(\xi,\eta)G_0(\xi,\tau;Q',0)G_0^*(\eta,\tau;q',0)\;. \tag{3.46}$$

For quantum mechanics the superpotential is

$$\mathcal{V}(\xi,\eta)=V(\xi)-V(\eta)=\lambda(\xi^4-\eta^4)\quad, \tag{3.47}$$

then

$$\begin{aligned}\mathcal{G}_1(\overrightarrow{Q},t;\overrightarrow{Q'},0) &= G_0^*(q,t;q',0)\int_0^t d\tau\int d\xi\; G_0(Q,t;\xi,\tau)V(\xi)G_0(\xi,\tau;Q',0) \qquad (3.48)\\ &- G_0(Q,t;Q',0)\int_0^t d\tau\int d\eta\; G_0^*(q,t;\eta,\tau)V(\eta)G_0^*(\eta,\tau;q',0)\;.\end{aligned}$$

At this point we need to know only the first space-time integral, since the second integral of the equation can be obtained from the first by the transformation, that is $(Q, Q' \to q, q')^*$. Let us write the integrand in a useful way

$$G_0(Q,t;\xi,\tau)G_0(\xi,\tau;Q',0) = \tag{3.49}$$
$$\left(\frac{m}{2\pi\hbar i}\right)\left(\frac{1}{t-\tau}\right)^{\frac{1}{2}}\left(\frac{1}{\tau}\right)^{\frac{1}{2}} exp\left[\gamma(\tau)+\beta(\tau)\xi-\alpha(\tau)\xi^2\right] ,$$

where we have defined

$$\gamma(\tau) = \frac{im}{2\hbar}\left(\frac{Q^2}{t-\tau}+\frac{Q'^2}{\tau}\right) , \tag{3.50}$$

$$\beta(\tau) = -\frac{im}{2\hbar}\left(\frac{2Q}{t-\tau}+\frac{2Q'}{\tau}\right) , \tag{3.51}$$

$$\alpha(\tau) = -\frac{im}{2\hbar}\left(\frac{1}{t-\tau}+\frac{1}{\tau}\right) , \tag{3.52}$$

The integral over space is simply a Gaussian integral

$$\begin{aligned}\int d\xi\; e^{(\beta(\tau)\xi\; - \;\alpha(\tau)\xi^2)}\;\lambda\xi^4 &= \lambda\frac{\partial^4}{\partial\beta^4}\int d\xi\; e^{(\beta(\tau)\xi\; - \;\alpha(\tau)\xi^2)} = \lambda\left(\frac{2\pi}{2\alpha}\right)^{\frac{1}{2}}\frac{\partial^4}{\partial\beta^4}\; e^{\frac{\beta^2}{4\alpha}} \\ &= \lambda(2\pi)^{\frac{1}{2}}\left(\frac{1}{2\alpha}\right)^{\frac{5}{2}}\left[3+6\left(\frac{\beta^2}{2\alpha}\right)+\left(\frac{\beta^2}{2\alpha}\right)^2\right]e^{\frac{\beta^2}{4\alpha}} \;. \end{aligned}\tag{3.53}$$

Now we have to do the integral over time, which is simply an integral of various powers of τ

$$\lambda\left(\frac{m}{\sqrt{2\pi\hbar i}}\right)\int_0^t d\tau\;\left(\frac{1}{t-\tau}\right)^{\frac{1}{2}}\left(\frac{1}{\tau}\right)^{\frac{1}{2}}\left(\frac{1}{2\alpha}\right)^{\frac{5}{2}}\left[3+6\left(\frac{\beta^2}{2\alpha}\right)+\left(\frac{\beta^2}{2\alpha}\right)^2\right]e^{\frac{\beta^2}{4\alpha}+\gamma} \;. \tag{3.54}$$

Since

$$\frac{\beta^2}{4\alpha}+\gamma=\frac{im}{2\hbar t}(Q-Q')^2 \quad , \tag{3.55}$$

$$\left(\frac{1}{t-\tau}\right)^{\frac{1}{2}}\left(\frac{1}{\tau}\right)^{\frac{1}{2}}\left(\frac{1}{2\alpha}\right)^{\frac{5}{2}}=\left(\frac{i\hbar}{mt}\right)^{\frac{5}{2}}(\tau(t-\tau))^2 \quad , \tag{3.56}$$

we can write

$$-\lambda\left(\frac{\hbar}{mt}\right)^2\left(\frac{m}{2\pi i\hbar t}\right)^{\frac{1}{2}}e^{\frac{im}{2\hbar t}(Q-Q')^2}\int_0^t d\tau \;\; (\tau(t-\tau))^2\left[3+6\left(\frac{\beta^2}{2\alpha}\right)+\left(\frac{\beta^2}{2\alpha}\right)^2\right] \quad , \tag{3.57}$$

i.e.

$$-\lambda\left(\frac{\hbar}{mt}\right)^2 G_0(Q,t;Q',0)\int_0^t d\tau \;\; (\tau(t-\tau))^2\left[3+6\left(\frac{\beta^2}{2\alpha}\right)+\left(\frac{\beta^2}{2\alpha}\right)^2\right] \quad . \tag{3.58}$$

The value of the integral is

$$\frac{t^5}{10}\left[1-2\left(\frac{m}{\hbar t}\right)^2(Q'^4+Q^4+Q'^3Q+Q'Q^3+Q'^2Q^2)-\frac{im}{\hbar t}(4Q'Q+3(Q'^2+Q^2))\right] \quad . \tag{3.59}$$

Finally, we write the complete expression for the first order propagator

$$\mathcal{G}_q(\overrightarrow{Q},t;\overrightarrow{Q'},0)=\mathcal{G}_0(\overrightarrow{Q},t;\overrightarrow{Q'},0)\Big(1+\lambda k(Q,Q';t)+\lambda k^*(q,q';t)\Big)+O(\lambda^2) \quad , \tag{3.60}$$

where

$$k(Q,Q';t)= \tag{3.61}$$
$$\frac{t^2}{10m}\left((4Q'Q+3(Q'^2+Q^2))+\left(\frac{2}{i\lambda_c ct}\right)(Q'^4+Q^4+Q'^3Q+Q'Q^3+Q'^2Q^2)\right) \quad ,$$

also we have defined the Compton wave length $\lambda_c=\frac{\hbar c}{mc^2}$. As remarkable result, we can see that for a quantum anharmonic oscillator we obtain a *separable superpropagator*.

3.5.2 Classical mechanics

Now we calculate the superpropagator to first order correction in the classical mechanics case. The difference is the change in the superpotential, that is

$$\mathcal{V}(\xi,\eta) = (\xi-\eta)V'\left(\frac{\xi+\eta}{2}\right) = \frac{\lambda}{2}(\xi^4-\eta^4+2(\xi^3\eta-\eta^3\xi)) \quad , \tag{3.62}$$

note that the first two terms on the right-hand are the same as in the quantum mechanics case, with the only difference that the coupling constant λ is divided by a factor two, the other terms are decidedly classical. Let us to calculate the latter:

$$\begin{aligned}\mathcal{G}_1(\overrightarrow{Q},t;\overrightarrow{Q'},0) &= \\ &\lambda\int_0^t d\tau\int d\xi G_0(Q,t;\xi,\tau)G_0(\xi,\tau;Q',0)\xi^3\int d\eta G_0^*(q,t;\eta,\tau)G_0^*(\eta,\tau;q',0)\eta \\ -&\lambda\int_0^t d\tau\int d\xi G_0(Q,t;\xi,\tau)G_0(\xi,\tau;Q',0)\xi\int d\eta G_0^*(q,t;\eta,\tau)G_0^*(\eta,\tau;q',0)\eta^3 \ .\end{aligned} \tag{3.63}$$

Similarly as the quantum calculation of the previous section, we need only one of the two integrals, of this equation since knowing one we can obtain the other with the transformation $(Q,Q'\to q,q')^*$. Firstly, we evaluate this integral

$$\begin{aligned}&\int d\xi\ G_0(Q,t;\xi,\tau)G_0(\xi,\tau;Q',0)\xi^3 = \\ &\left(\frac{m}{2\pi\hbar i}\right)\left(\frac{1}{t-\tau}\right)^{\frac{1}{2}}\left(\frac{1}{\tau}\right)^{\frac{1}{2}}e^{\gamma(\tau)}\int d\xi\ e^{(\beta(\tau)\xi\ -\ \alpha(\tau)\xi^2)}\xi^3 \quad .\end{aligned} \tag{3.64}$$

As in the previous section, we have to calculate a Gaussian integral

$$\begin{aligned}\int d\xi\ e^{(\beta(\tau)\xi\ -\ \alpha(\tau)\xi^2)}\xi^3 &= \frac{\partial^3}{\partial\beta^3}\int d\xi\ e^{(\beta(\tau)\xi\ -\ \alpha(\tau)\xi^2)} = \left(\frac{2\pi}{2\alpha}\right)^{\frac{1}{2}}\frac{\partial^3}{\partial\beta^3}\ e^{\frac{\beta^2}{4\alpha}+\gamma} \\ &= (2\pi)^{\frac{1}{2}}\left(\frac{1}{2\alpha}\right)^{\frac{5}{2}}\beta\left[3+\frac{\beta^2}{2\alpha}\right]e^{\frac{\beta^2}{4\alpha}+\gamma} \quad .\end{aligned} \tag{3.65}$$

Secondly, we evaluate

$$\int d\eta\; G_0^*(q,t;\eta,\tau)G_0^*(\eta,\tau;q',0)\eta = \tag{3.66}$$

$$\left(\frac{m}{2\pi\hbar(-i)}\right)\left(\frac{1}{t-\tau}\right)^{\frac{1}{2}}\left(\frac{1}{\tau}\right)^{\frac{1}{2}} e^{\gamma^*(\tau)}\int d\eta\; e^{(\beta^*(\tau)\xi\;-\;\alpha^*(\tau)\eta^2)}\eta \quad .$$

Even in this case, we have need only another Gaussian integral

$$\int d\eta\; e^{(\beta^*(\tau)\xi\;-\;\alpha^*(\tau)\eta^2)}\eta = (2\pi)^{\frac{1}{2}}\left(\frac{1}{2\alpha^*}\right)^{\frac{3}{2}}\beta^* e^{(\frac{\beta^2}{4\alpha})^*+\gamma^*} \quad , \tag{3.67}$$

where

$$\beta^*(\tau) = \frac{im}{\hbar}\left(\frac{q}{t-\tau}+\frac{q'}{\tau}\right) \quad , \tag{3.68}$$

$$\alpha^*(\tau) = \frac{im}{2\hbar}\left(\frac{1}{t-\tau}+\frac{1}{\tau}\right) \quad . \tag{3.69}$$

Finally, we calculate the integral over time, which is simply an integral of various powers of the time variable

$$\lambda(2\pi)\left(\frac{m}{2\pi\hbar i}\right)\left(\frac{m}{2\pi\hbar(-i)}\right) e^{\frac{\beta^2}{4\alpha}+\gamma} e^{(\frac{\beta^2}{4\alpha})^*+\gamma^*} \tag{3.70}$$

$$\times \quad \int_0^t d\tau \left(\frac{1}{t-\tau}\right)\left(\frac{1}{\tau}\right)\left(\frac{1}{2\alpha}\right)^{\frac{5}{2}}\beta\left[3+\frac{\beta^2}{2\alpha}\right]\left(\frac{1}{2\alpha^*}\right)^{\frac{3}{2}}\beta^* \quad .$$

Since

$$\frac{\beta^2}{4\alpha}+\gamma = \frac{im}{2\hbar t}(Q-Q')^2 \quad , \tag{3.71}$$

$$(\frac{\beta^2}{4\alpha})^*+\gamma^* = -\frac{im}{2\hbar t}(q'-q)^2 \quad , \tag{3.72}$$

$$\beta\left[3+\frac{\beta^2}{2\alpha}\right] = -\frac{im}{\hbar}\left(\frac{Q}{t-\tau}+\frac{Q'}{\tau}\right)\left[3-\frac{im}{\hbar t}\left(Q^2\frac{\tau}{t-\tau}+Q'^2\frac{t-\tau}{\tau}+2QQ'\right)\right] \quad , \tag{3.73}$$

we can write

$$
\begin{aligned}
& i\lambda \left(\frac{\hbar}{mt^3}\right) \mathcal{G}_0(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0) \\
\times\ & \int_0^t d\tau\, (\tau(t-\tau))^3 \left(\frac{Q}{t-\tau} + \frac{Q'}{\tau}\right) \left(\frac{q}{t-\tau} + \frac{q'}{\tau}\right) \left[3 - \frac{im}{\hbar t}\left(Q^2 \frac{\tau}{t-\tau} + Q'^2 \frac{t-\tau}{\tau} + 2QQ'\right)\right] \quad .
\end{aligned}
\tag{3.74}
$$

This integral is equal to

$$
\begin{aligned}
& \frac{3}{10} t^5 \left(\frac{Qq + Q'q'}{2} + \frac{Qq' + Q'q}{3}\right) \\
& -i\frac{mt^4}{10\hbar}\left(Q^3(2q + \frac{1}{2}q') + Q^2Q'(\frac{3}{2}q + q') + QQ'^2(q + \frac{3}{2}q') + Q'^3(\frac{1}{2}q + 2q')\right) \quad .
\end{aligned}
\tag{3.75}
$$

Finally, we arrive at the espression for the first order propagator

$$
\begin{aligned}
& \mathcal{G}_c(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0) = \frac{1}{2}\mathcal{G}_q(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0) + \\
& \mathcal{G}_0(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0)\Big[1 + \lambda\big(h(Q, q, Q', q'; t) + g(Q, q, Q', q'; t) + g^*(q, Q, q', Q'; t)\big)\Big] + O(\lambda^2) \quad ,
\end{aligned}
\tag{3.76}
$$

where

$$
h(Q, q, Q', q'; t) = \frac{6t^2}{10m}\left(\frac{Qq + Q'q'}{2} + \frac{Qq' + Q'q}{3}\right) \quad , \tag{3.77}
$$

$$
\begin{aligned}
& g(Q, q, Q', q'; t) = \\
& \frac{t}{10i\hbar}\left(Q^3(2q + \frac{1}{2}q') + Q^2Q'(\frac{3}{2}q + q') + QQ'^2(q + \frac{3}{2}q') + Q'^3(\frac{1}{2}q + 2q')\right) \quad .
\end{aligned}
\tag{3.78}
$$

As expected, we obtain a *nonseparable superpropagator*. We remark that this result is a consequence of the coupling, incorporated in our Liouville space description of the classical dynamics, of the Hilbert space and its dual. As another result, we note that the perturbative expansion turns out to be a short-time expansion, indeed in both cases (quantum and classical) we have a linear and also a quadratic dependence in time of the corrections.

3.6 Plane wave evolution

In this section, we study the evolution in time for a density matrix in the case of a pure state, presenting a plane wave. The general equation (2.101), which describes the evolution in time for a density matrix is

$$\langle\langle Q, q|\rho(t)\rangle\rangle = \int dQ' dq' \mathcal{G}(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0)\langle\langle Q', q'|\rho(0)\rangle\rangle \quad , \tag{3.79}$$

which we evaluate again for the anharmonic oscillator treated in Section 3.5. Let

$$\langle\langle Q', q'|\rho(0)\rangle\rangle = \rho(Q', q'; 0) = \frac{1}{2\pi\hbar} e^{\frac{ip}{\hbar}(Q'-q')} \quad , \tag{3.80}$$

be the initial value for the matrix elements. We want to see what happens in the evolution and to compare the classical and quantum evolutions for this system in perturbation theory.

3.6.1 Quantum evolution

We consider in this case the quantum superpropagator calculated in the previous section, which is

$$\mathcal{G}_q(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0) = \mathcal{G}_0(\overrightarrow{Q}, t; \overrightarrow{Q'}, 0)\Big(1 + \lambda k(Q, Q'; t) + \lambda k^*(q, q'; t)\Big) \quad , \tag{3.81}$$

where the subscript q means quantum, and

$$k(Q, Q'; t) = \frac{t^2}{10m}\left((4Q'Q + 3(Q'^2 + Q^2)) + \left(\frac{2}{i\lambda_c ct}\right)(Q'^4 + Q^4 + Q'^3 Q + Q'Q^3 + Q'^2 Q^2)\right) \quad .$$

So we need the following integrals:

$$f_0(Q, t) \equiv \int dQ' \; C e^{i\alpha(Q'-Q)^2 \; + \; i\frac{p}{\hbar}Q'} = \frac{e^{i\frac{p}{\hbar}Q}}{(2\pi\hbar)^{\frac{1}{2}}} e^{-i\frac{p^2}{2m\hbar}t} \quad , \tag{3.82}$$

where $C = \left(\frac{m}{2\pi\hbar i t}\right)^{\frac{1}{2}}$, and $\alpha = \frac{m}{2\hbar t}$.

$$f_0(Q, t) f_1(Q, t) \equiv \int dQ' \; C e^{i\alpha(Q'-Q)^2 \; + \; i\frac{p}{\hbar}Q'} Q' = \frac{e^{i\frac{p}{\hbar}Q}}{(2\pi\hbar)^{\frac{1}{2}}} e^{-i\frac{p^2}{2m\hbar}t}\left(Q - \frac{pt}{m}\right) \quad , \tag{3.83}$$

$$f_0(Q,t)f_2(Q,t) \equiv \int dQ'\ Ce^{i\alpha(Q'-Q)^2\ +\ i\frac{p}{\hbar}Q'}Q'^2 =$$

$$= \frac{e^{i\frac{p}{\hbar}Q}}{(2\pi\hbar)^{\frac{1}{2}}}e^{-i\frac{p^2}{2m\hbar}t}\left(Q^2 + 2Q(Q-\frac{pt}{m}) + \frac{i\hbar t}{m} + \left(\frac{pt}{m}\right)^2\right)\quad , \tag{3.84}$$

$$f_0(Q,t)f_3(Q,t) \equiv \int dQ'\ Ce^{i\alpha(Q'-Q)^2\ +\ i\frac{p}{\hbar}Q'}Q'^3 = \frac{e^{i\frac{p}{\hbar}Q}}{(2\pi\hbar)^{\frac{1}{2}}}e^{-i\frac{p^2}{2m\hbar}t}\times \tag{3.85}$$

$$\left[\frac{3\hbar p}{im^2}t^2 - (\frac{pt}{m})^3 + Q^3 + 3Q\left(Q^2 + 2Q(Q-\frac{pt}{m}) + \frac{i\hbar t}{m} + \left(\frac{pt}{m}\right)^2\right) + 3Q^2(Q-\frac{pt}{m})\right]\quad ,$$

$$f_0(Q,t)f_4(Q,t) \equiv \int dQ'\ Ce^{i\alpha(Q'-Q)^2\ +\ i\frac{p}{\hbar}Q'}Q'^4 = \frac{e^{i\frac{p}{\hbar}Q}}{(2\pi\hbar)^{\frac{1}{2}}}e^{-i\frac{p^2}{2m\hbar}t}\times$$

$$\Big[\ \left(3 + \frac{6p^2}{im\hbar}t + (\frac{p^2}{im\hbar})^2t^2\right)\left(\frac{i\hbar t}{m}\right)^2 + Q^4 +$$

$$+4Q\Big[\frac{3\hbar p}{im^2}t^2 - (\frac{pt}{m})^3 + Q^3 + 3Q\left(Q^2 + 2Q(Q-\frac{pt}{m}) + \frac{i\hbar t}{m} + \left(\frac{pt}{m}\right)^2\right) + 3Q^2(Q-\frac{pt}{m})\Big]$$

$$4Q^3(Q-\frac{pt}{m}) + 6Q^2\left(Q^2 + 2Q(Q-\frac{pt}{m}) + \frac{i\hbar t}{m} + \left(\frac{pt}{m}\right)^2\right)\Big]\quad . \tag{3.86}$$

It is important to observe that $f_0(Q,t)f_0^*(q,t) = \rho(Q,q;0)$; then, we can write down the density matrix at time t

$$
\begin{aligned}
\rho(Q,q;t) &= \rho(Q,q;0)\Big[1+\frac{\lambda t^2}{10m}\Big[\big(4Qf_1(Q,t)+3Q^2+3f_2(Q,t)\big)\\
&+ \frac{2}{i\lambda_c ct}\big(Q^4+f_4(Q,t)+Qf_3(Q,t)+Q^3f_1(Q,t)+Q^2f_2(Q,t)\big)\\
&+ \big(4qf_1^*(q,t)+3q^2+3f_2^*(q,t)\big)\\
&- \frac{2}{i\lambda_c ct}\big(q^4+f_4^*(q,t)+qf_3^*(q,t)+q^3f_1^*(q,t)+q^2f_2^*(q,t)\big)\Big]\Big] \quad . \qquad (3.87)
\end{aligned}
$$

This lengthy expression can be much simplified, if we calculate all the terms explicity. We write the real and the imaginary part of the density matrix

$$
\begin{aligned}
\mathrm{Re}\rho(Q,q;t) &= \frac{\cos[\frac{p}{\hbar}(Q-q)]}{2\pi\hbar}\\
&+ \frac{\lambda t^2}{20\pi\hbar m}\Big[\cos[\frac{p}{\hbar}(Q-q)]\Big(60(Q^2+q^2)-40\frac{pt}{m}(Q+q)+18\left(\frac{pt}{m}\right)^2\Big)\Big]\\
&+ \frac{\lambda t^2}{20\pi\hbar m}\frac{2}{\lambda_c ct}\Big[\sin[\frac{p}{\hbar}(Q-q)]\Big(93(Q^4-q^4)-64\frac{pt}{m}(Q^3-q^3)\Big]\\
&+ \frac{\lambda t^2}{20\pi\hbar m}\frac{2}{\lambda_c ct}\Big[\sin[\frac{p}{\hbar}(Q-q)]\Big(18\Big(\frac{pt}{m}\Big)^2(Q^2-q^2)-5\Big(\frac{pt}{m}\Big)^3(Q-q)\Big)\Big] \quad ,
\end{aligned}
$$

(3.88)

$$
\begin{aligned}
\mathrm{Im}\rho(Q,q;t) &= \frac{\sin[\frac{p}{\hbar}(Q-q)]}{2\pi\hbar}\\
&+ \frac{\lambda t^2}{20\pi\hbar m}\Big[\sin[\frac{p}{\hbar}(Q-q)]\Big(60(Q^2+q^2)-40\frac{pt}{m}(Q+q)+18\left(\frac{pt}{m}\right)^2\Big)\Big]\\
&- \frac{\lambda t^2}{20\pi\hbar m}\frac{2}{\lambda_c ct}\Big[\cos[\frac{p}{\hbar}(Q-q)]\Big(93(Q^4-q^4)-64\frac{pt}{m}(Q^3-q^3)\Big]\\
&- \frac{\lambda t^2}{20\pi\hbar m}\frac{2}{\lambda_c ct}\Big[\cos[\frac{p}{\hbar}(Q-q)]\Big(18\Big(\frac{pt}{m}\Big)^2(Q^2-q^2)-5\Big(\frac{pt}{m}\Big)^3(Q-q)\Big)\Big] \quad .
\end{aligned}
$$

(3.89)

3.6.2 Classical evolution

We consider here the classical superpropagator. The treatment is the same as developed in the previous subsection 3.6.1:

$$\begin{aligned} \mathcal{G}_c(\overrightarrow{Q},t;\overrightarrow{Q'},0) &= \frac{1}{2}\mathcal{G}_q(\overrightarrow{Q},t;\overrightarrow{Q'},0) \\ &+ \mathcal{G}_0(\overrightarrow{Q},t;\overrightarrow{Q'},0)\Big[1+\lambda\Big(h(Q,q,Q',q';t)+g(Q,q,Q',q';t)+g^*(q,Q,q',Q';t)\Big)\Big] \quad , \end{aligned}$$

where

$$h(Q,q,Q',q';t) = \frac{6t^2}{10m}\left(\frac{Qq+Q'q'}{2}+\frac{Qq'+Q'q}{3}\right) \quad , \tag{3.90}$$

$$g(Q,q,Q',q';t) = \frac{t}{10i\hbar}\left(Q^3(2q+\frac{1}{2}q')+Q^2Q'(\frac{3}{2}q+q')+QQ'^2(q+\frac{3}{2}q')+Q'^3(\frac{1}{2}q+2q')\right) \quad . \tag{3.91}$$

Using the integrals give in the previous subsection, we can immediately write down the density matrix at time t

$$\begin{aligned} \rho_c(Q,q;t) &= \frac{1}{2}\rho_q(Q,q;t) \\ &+ \rho(Q,q;0)\left[1+\frac{6t^2}{10m}\left(\frac{Qq}{2}+\frac{1}{2}f_1(Q,t)f_1^*(q,t)+\frac{1}{3}qf_1(Q,t)+\frac{1}{3}Qf_1^*(q,t)\right)\right] \\ &+ \rho(Q,q;0)\left[\frac{t}{10i\hbar}\left(Q^3(2q+\frac{1}{2}f_1^*(q,t))+Q^2f_1(Q,t)(\frac{3}{2}q+f_1^*(q,t))\right)\right] \\ &+ \rho(Q,q;0)\left[\frac{t}{10i\hbar}\left(Qf_2(Q,t)(q+\frac{3}{2}f_1^*(q,t))+f_3(Q,t)(\frac{1}{2}q+2f_1^*(q,t))\right)\right] \\ &+ \rho(Q,q;0)\left[\frac{it}{10\hbar}\left(q^3(2Q+\frac{1}{2}f_1(Q,t))+q^2f_1^*(q,t)(\frac{3}{2}Q+f_1(Q,t))\right)\right] \\ &+ \rho(Q,q;0)\left[\frac{it}{10\hbar}\left(qf_2^*(q,t)(Q+\frac{3}{2}f_1(Q,t))+f_3^*(q,t)(\frac{1}{2}Q+2f_1(Q,t))\right)\right] \\ &. \end{aligned} \tag{3.92}$$

Like the quantum calculation, this lengthy expression can be simplified, if we calculate all the terms explicity. We write the real and the imaginary part of the density matrix

$$
\begin{aligned}
\mathrm{Re}\rho(Q,q;t) &= \frac{\cos[\frac{p}{\hbar}(Q-q)]}{2\pi\hbar} + \\
&+ \frac{\lambda t^2}{20\pi\hbar m}\Big[\cos[\frac{p}{\hbar}(Q-q)]\Big(30(Q^2+q^2+Qq) - 40\frac{pt}{m}(Q+q) + 26\left(\frac{pt}{m}\right)^2\Big)\Big] \\
&+ \frac{\lambda t^2}{20\pi\hbar m}\frac{2}{\lambda_c ct}\Big[\sin[\frac{p}{\hbar}(Q-q)]\Big(93(Q^4-q^4) - 96\frac{pt}{m}(Q^3-q^3)\Big] \\
&+ \frac{\lambda t^2}{20\pi\hbar m}\frac{2}{\lambda_c ct}\Big[\sin[\frac{p}{\hbar}(Q-q)]\Big(40\Big(\frac{pt}{m}\Big)^2(Q^2-q^2) - 15\Big(\frac{pt}{m}\Big)^3(Q-q)\Big)\Big] \\
&+ \frac{\lambda t^2}{20\pi\hbar m}\frac{2}{\lambda_c ct}\Big[\sin[\frac{p}{\hbar}(Q-q)]\Big(41(Q^3q-q^3Q) - 60\frac{pt}{m}(Q^2q-q^2Q)\Big)\Big]
\end{aligned}
\tag{3.93}
$$

$$
\begin{aligned}
\mathrm{Im}\rho(Q,q;t) &= \frac{\sin[\frac{p}{\hbar}(Q-q)]}{2\pi\hbar} + \\
&+ \frac{\lambda t^2}{20\pi\hbar m}\Big[\sin[\frac{p}{\hbar}(Q-q)]\Big(30(Q^2+q^2+Qq) - 40\frac{pt}{m}(Q+q) + 26\left(\frac{pt}{m}\right)^2\Big)\Big] \\
&- \frac{\lambda t^2}{20\pi\hbar m}\frac{2}{\lambda_c ct}\Big[\cos[\frac{p}{\hbar}(Q-q)]\Big(93(Q^4-q^4) - 96\frac{pt}{m}(Q^3-q^3)\Big] \\
&- \frac{\lambda t^2}{20\pi\hbar m}\frac{2}{\lambda_c ct}\Big[\cos[\frac{p}{\hbar}(Q-q)]\Big(40\Big(\frac{pt}{m}\Big)^2(Q^2-q^2) - 15\Big(\frac{pt}{m}\Big)^3(Q-q)\Big)\Big] \\
&- \frac{\lambda t^2}{20\pi\hbar m}\frac{2}{\lambda_c ct}\Big[\cos[\frac{p}{\hbar}(Q-q)]\Big(41(Q^3q-q^3Q) - 60\frac{pt}{m}(Q^2q-q^2Q)\Big)\Big] \quad .
\end{aligned}
\tag{3.94}
$$

In the following, we illustrate graphically the results obtained for these evolutions. We have fixed the mass of the particle $m = 0.5\mathrm{MeV}$, the velocity $v = 10^{-5}\mathrm{m/s}$, the time interval $t = 10^{-7}\mathrm{s}$ and the coupling constant $\lambda = 1eV/1.8\mathrm{m}^4$. The Q, q coordinates are expressed in meters. We do not want to give a quantitative study, since this is only an illustration of how the path integral theory can be used and the model is not realistic. However, by this qualitative study, we can learn that the perturbation theory works well up to where the curvature of the superpotentials becomes noticeable, which happens in this case at

1×10^{-3}m. In this way, we convince ourself indirectly that the perturbative expansion is a short-time expansion. For the time interval $t = 10^{-6}$s the first order correction becomes of the same order of magnitude of the leading term; then we cannot trust in the expansion. We see in Fig. 3.2 the contourplot of the initial real part of the density matrix (times $2\pi\hbar$), which is approximately constant and equal to one. The Fig. 3.3 shows the initial imaginary part of the density matrix (times $2\pi\hbar$), in units of $\hbar$/m. The Fig. 3.4 - 3.5 show, respectively, the quantum and classical superpotentials, which present a noticeable curvature at 1×10^{-3}m. The Fig. 3.6 - 3.7 show, respectively, the imaginary and real first order correction for the quantum and classical dynamics. Finally, we show in Fig. 3.8 the comparison of imaginary and real first order correction for the quantum and classical dynamics.

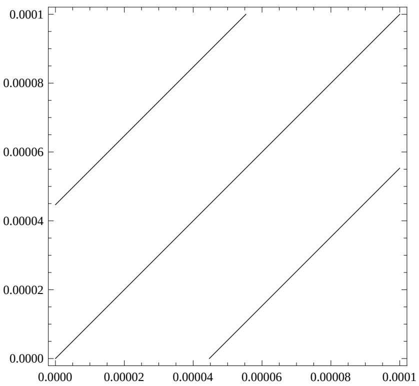

Figure 3.2: Initial real part of the density matrix times $(2\pi\hbar)$. The differences between the lines in this contour plot are in absolute value 1×10^{-11}, implying that the real part is approximately constant and equal to 1 in this region of the coordinates.

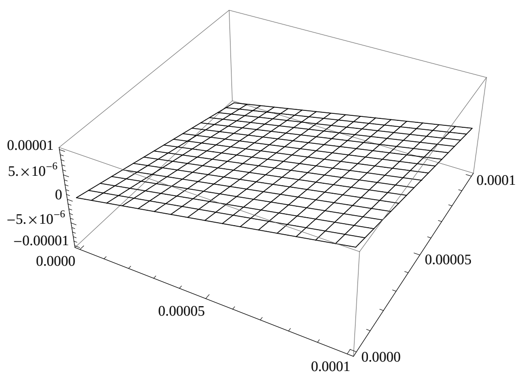

Figure 3.3: Initial imaginary part of the density matrix (times $2\pi\hbar$), in units of $\hbar$/m

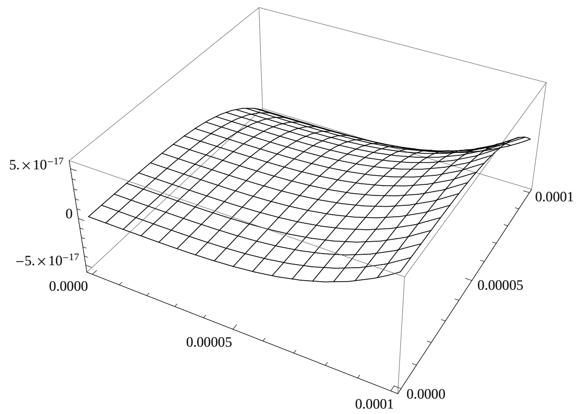

Figure 3.4: Quantum superpotential, in units of eV.

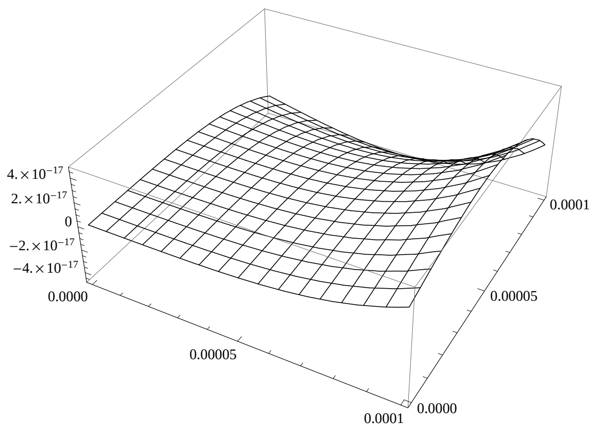

Figure 3.5: Classical superpotential, in units of eV.

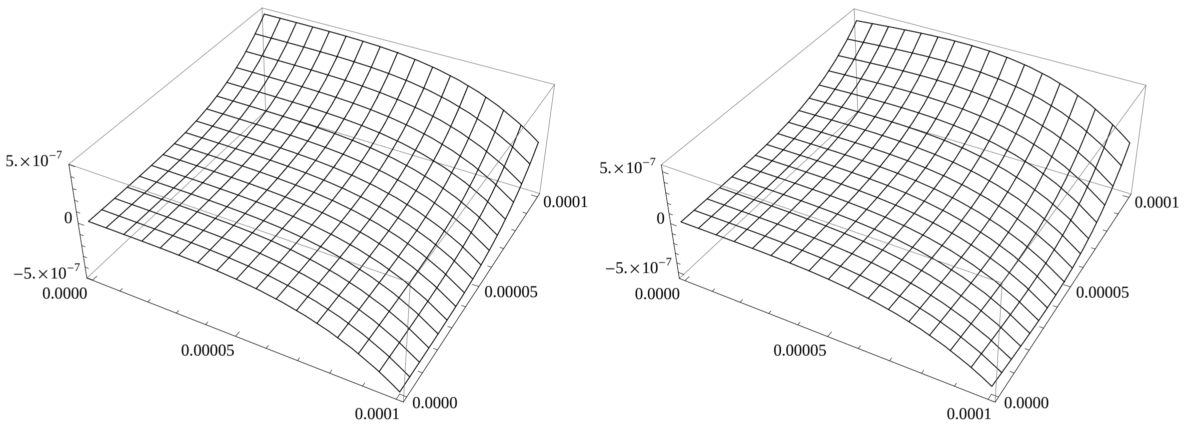

Figure 3.6: The left figure shows the imaginary part of the quantum first order correction, the right one the corresponding classical term (times $2\pi\hbar$), in units of $\hbar$/m .

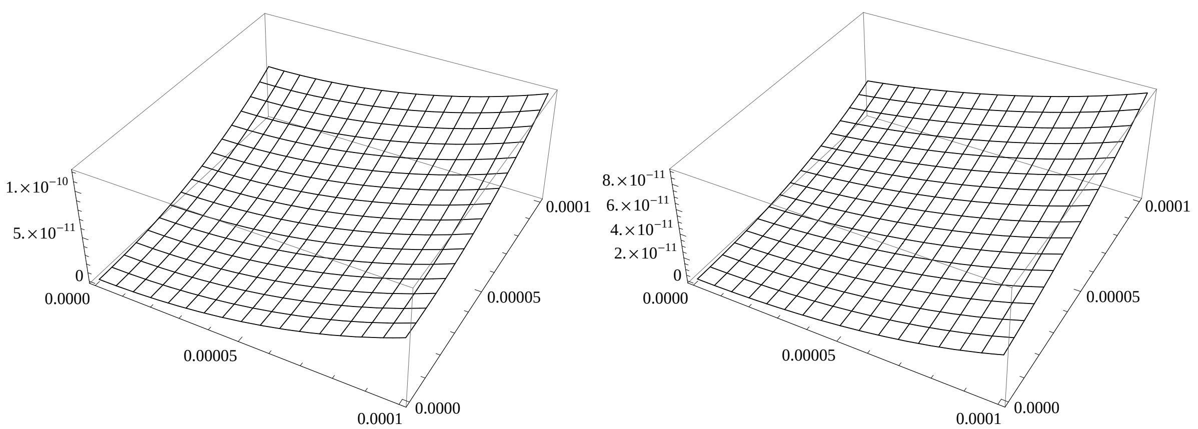

Figure 3.7: The left figure shows the real part of the quantum first order correction, the right one the corresponding classical term (times $2\pi\hbar$), in units of $\hbar$/m .

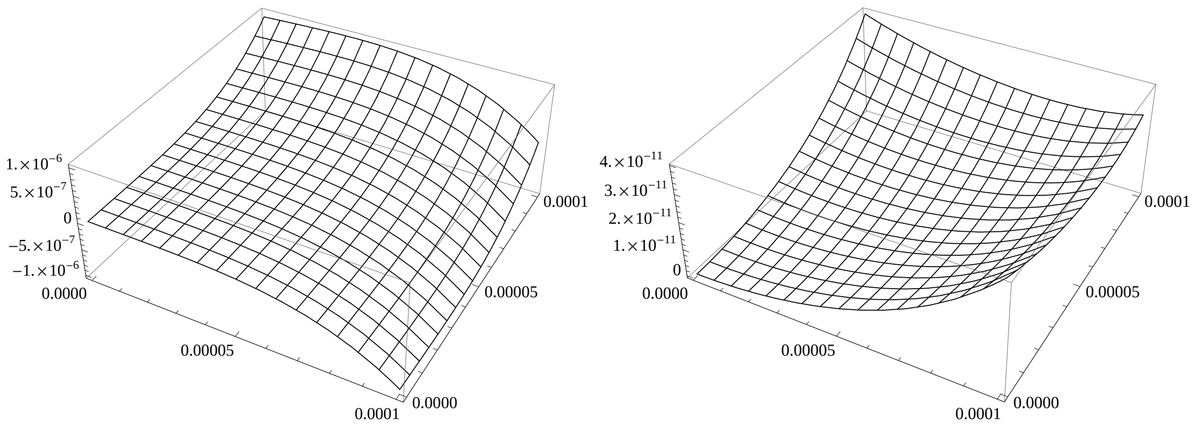

Figure 3.8: The left figure shows the imaginary part of the quantum minus classical first order correction, the right one the real part of the quantum minus classical first order correction (times $2\pi\hbar$), in units of $\hbar$/m .

Chapter 4

Two-particle entanglement

This chapter is an exstension, of what we have done previously, to the case of two massive particles. Here, we use these results with the objective of investigating about entanglement properties of the system.

4.1 Two-particle Liouville equation

In this section, we rewrite the Liouville equation (2.37) for the case of two massive particles. Let H be the Hamiltonian for two particles which interact with a potential depending only on the distance between the particles

$$H(p_1, p_2; x_1, x_2) = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(x_1 - x_2) \quad . \tag{4.1}$$

The Liouville equation (2.37) becomes

$$\begin{aligned} -\partial_t \rho &= \frac{\partial H}{\partial p_1}\frac{\partial \rho}{\partial x_1} - \frac{\partial H}{\partial x_1}\frac{\partial \rho}{\partial p_1} + \frac{\partial H}{\partial p_2}\frac{\partial \rho}{\partial x_2} - \frac{\partial H}{\partial x_2}\frac{\partial \rho}{\partial p_2} \\ &= (\frac{p_1}{m_1}\frac{\partial}{\partial x_1} + \frac{p_2}{m_2}\frac{\partial}{\partial x_2} - \frac{\partial V}{\partial x_1}\frac{\partial}{\partial p_1} - \frac{\partial V}{\partial x_2}\frac{\partial}{\partial p_2})\rho \quad , \end{aligned} \tag{4.2}$$

using the following Fourier transform

$$\rho(x_1, x_2; y_1, y_2) = \int dp_1 dp_2 \; e^{ip_1 y_1 + ip_2 y_2} \rho(x_1, x_2; p_1, p_2) \quad , \tag{4.3}$$

we obtain this equation

$$-i\partial_t\rho(x_1,x_2;y_1,y_2) = (\frac{1}{m_1}\frac{\partial}{\partial y_1}\frac{\partial}{\partial x_1} + \frac{1}{m_2}\frac{\partial}{\partial y_2}\frac{\partial}{\partial x_2} - y_1\frac{\partial V}{\partial x_1} - y_2\frac{\partial V}{\partial x_2})\rho(x_1,x_2;y_1,y_2) \quad . \quad (4.4)$$

Now, in analogy with the Sec. (2.3), we use the following transformation

$$Q_i = x_i + \frac{y_i}{2} \quad , \quad q_i = x_i - \frac{y_i}{2} \quad , \qquad i = 1,2. \qquad (4.5)$$

This lead us to the following form of the Liouville equation

$$i\partial_t\rho(Q_1,Q_2,q_1,q_2) = (H(Q_1,Q_2) - H(q_1,q_2) + \mathcal{E}(Q_1,Q_2;q_1,q_2))\rho(Q_1,Q_2,q_1,q_2) \qquad (4.6)$$

where

$$H(Q_1,Q_2) = -\frac{1}{2m_1}\partial^2_{Q_1^2} - \frac{1}{2m_2}\partial^2_{Q_2^2} + V(Q_1 - Q_2) \quad , \qquad (4.7)$$

$$H(q_1,q_2) = -\frac{1}{2m_1}\partial^2_{q_1^2} - \frac{1}{2m_2}\partial^2_{q_2^2} + V(q_1 - q_2) \quad , \qquad (4.8)$$

$$\begin{aligned} \mathcal{E}(Q_1,Q_2;q_1,q_2) &= (Q_1 - q_1)\partial_1 V\left(\frac{Q_1+q_1}{2} - \frac{Q_2+q_2}{2}\right) \\ &+ (Q_2 - q_2)\partial_2 V\left(\frac{Q_1+q_1}{2} - \frac{Q_2+q_2}{2}\right) \\ &+ V(q_1 - q_2) - V(Q_1 - Q_2) \quad , \qquad (4.9) \end{aligned}$$

where $\partial_i = \partial_{\frac{Q_i+q_i}{2}}$ for $i = 1,2$.

4.2 Path integral

As developed in Section 2.5, again we generalize the path integral on Liouville space for the case of two massive particles. The main step is to write a super-Hamiltonian that reproduces the Liouville equation (4.6). Therefore, straightforwardly we write

$$\langle\langle Q_1, Q_2, q_1, q_2|\mathcal{H}'|Q_1', Q_2', q_1', q_2'\rangle\rangle =$$
$$\mathcal{H}(Q_1, Q_2, q_1, q_2, Q_1', Q_2', q_1', q_2') + \mathcal{E}(Q_1, Q_2, q_1, q_2, Q_1', Q_2', q_1', q_2') \ =$$
$$\delta(Q_1 - Q_1')\delta(q_1 - q_1')\delta(Q_2 - Q_2')\delta(q_2 - q_2')(H(Q_1, Q_2) - H(q_1, q_2) + \mathcal{E}(Q_1, Q_2; q_1, q_2)) \quad . \tag{4.10}$$

Doing the same steps developed in Section 2.5, we can write down the expression for the superpropagator

$$\mathcal{G}(\overrightarrow{Q_1}, \overrightarrow{Q_2}, t; \overrightarrow{Q_1'}, \overrightarrow{Q_2'}, 0) = \int \mathcal{D}[\overrightarrow{Q_1}]\mathcal{D}[\overrightarrow{Q_2}] \ e^{\frac{i}{\hbar}\mathcal{S}[\overrightarrow{Q_1}, \overrightarrow{Q_2}]} \quad . \tag{4.11}$$

These integrals have the boundary conditions $\overrightarrow{Q_1}(t) = \overrightarrow{Q_1} = (Q_1, q_1)$, $\overrightarrow{Q_1}(0) = \overrightarrow{Q_1'} = (Q_1', q_1')$, $\overrightarrow{Q_2}(t) = \overrightarrow{Q_2} = (Q_2, q_2)$, $\overrightarrow{Q_2}(0) = \overrightarrow{Q_2'} = (Q_2', q_2')$ and $\mathcal{S}$ is the superaction:

$$\mathcal{S} = \int d\tau(\mathcal{T}(\dot{Q}_1, \dot{Q}_2, \dot{q}_1, \dot{q}_2) - \mathcal{V}(Q_1, Q_2, q_1, q_2)) = \int d\tau \mathcal{L}(\dot{Q}_1, \dot{Q}_2, \dot{q}_2, \dot{q}_1, Q_1, Q_2, q_1, q_2) \quad . \tag{4.12}$$

Finally, we arrive at the evolution equation for the two-particle density matrix in the form

$$\langle\langle Q_1, Q_2, q_1, q_2|\rho(t)\rangle\rangle =$$
$$\int dQ_1' dQ_2' dq_1' dq_2' \int \mathcal{D}[\overrightarrow{Q_1}]\mathcal{D}[\overrightarrow{Q_2}] \ e^{\frac{i}{\hbar}\mathcal{S}[\overrightarrow{Q_1}, \overrightarrow{Q_2}]}\langle\langle Q_1', Q_2', q_1', q_2'|\rho(0)\rangle\rangle \quad . \tag{4.13}$$

4.3 Perturbative expansion

In order to study the evolution of the density matrix when there are interactions that we cannot treat exactly, even for two particles, it takes a few steps to generalize the perturbative expansion developed in Section 3.4. Here we write only the main results. Firstly we consider the superpropagator

$$\mathcal{G}(\overrightarrow{Q_1}, \overrightarrow{Q_2}, t; \overrightarrow{Q_1'}, \overrightarrow{Q_2'}, 0) = \int \mathcal{D}[\overrightarrow{Q_1}]\mathcal{D}[\overrightarrow{Q_2}] \ e^{\frac{i}{\hbar}\mathcal{T}(\dot{\overrightarrow{Q_1}}, \dot{\overrightarrow{Q_2}})}e^{-\frac{i}{\hbar}\mathcal{V}(\overrightarrow{Q_1}, \overrightarrow{Q_2})} \quad , \tag{4.14}$$

secondly, we expand the superpotential term into a power series, using a formula for the

N-th power of the integral. Finally considering individual terms of the expansion, we sum these terms and write down the pertubation theory in the form of a Dyson integral equation for the full superpropagator

$$\mathcal{G}(\overrightarrow{Q}_1, \overrightarrow{Q}_2, t; \overrightarrow{Q'}_1, \overrightarrow{Q'}_2, 0) = \mathcal{G}_0(\overrightarrow{Q}_1, \overrightarrow{Q}_2, t; \overrightarrow{Q'}_1, \overrightarrow{Q'}_2, 0) \tag{4.15}$$
$$-\frac{i}{\hbar}\int_0^t d\tau \int d\overrightarrow{\zeta}_1 d\overrightarrow{\zeta}_2\, \mathcal{G}_0(\overrightarrow{Q}_1, \overrightarrow{Q}_2, t; \overrightarrow{\zeta}_1, \overrightarrow{\zeta}_2, \tau)\mathcal{V}(\overrightarrow{\zeta}_1, \overrightarrow{\zeta}_2)\mathcal{G}(\overrightarrow{\zeta}_1, \overrightarrow{\zeta}_2, \tau; \overrightarrow{Q'}_1, \overrightarrow{Q'}_2, 0) \ \ ,$$

where $\overrightarrow{\zeta}_1 = (\xi_1, \eta_1)$ and $\overrightarrow{\zeta}_2 = (\xi_2, \eta_2)$.

4.4 Entanglement

What we have done in this chapter so far, is useful to study the entanglement between two particles. Here, we give only a general idea of how this can be done. Despite the common idea that the entanglement is a property only of quantum mechanical systems, we argue that we can find another form of entanglement for classical systems. Let two particles initially be in a product state, say uncorrelated, then we can write their initial density matrix as

$$\rho(0) = \rho_1(0) \otimes \rho_2(0) \ \ . \tag{4.16}$$

Thanks to the our path integral formulation of the classical and quantum dynamics we can follow the evolution of the density matrix in time. The resulting density matrix, in general, will not be just the product of the two density matrices as in the initial state, and we can quantify the entanglement by the reduced density matrix

$$\rho_1(t) \equiv \mathrm{Tr}_2[\rho(t)] \ \ , \tag{4.17}$$

and by evaluating, for example, the linear entropy defined as

$$S_{lin} \equiv 1 - \mathcal{P}(t) \ \ , \tag{4.18}$$

where $\mathcal{P}(t) \equiv Tr[\rho_1(t)^2]$ is called purity. The purity is equals one for pure factorizable two-particle states; correspondingly, the linear entrpy is zero, in this case. Therefore, if $\mathcal{P} \neq 1$, the state is not factorizable. If the impurity or non-zero entropy is generated by the interactions in the two-particle system, this is called *dynamically assisted entanglement generation* [13]. For example, if we consider an interaction between two particles by an anharmonic oscillator [7], we may have uncorrelated particles at an initial time. In the presence of their interacting potential, we can calculate the evolving density matrix, with the help of the perturbative expansion. Furthermore, we can distinguish classical and quantum mechanical evolution through a different superpotential, which is for the quantum case a separable superpotential

$$\mathcal{V}(Q_1, Q_2; q_1, q_2) = V(Q_1, Q_2) - V(q_1, q_2) = \lambda\Big((Q_1 - Q_2)^4 - (q_1 - q_2)^4\Big) \quad , \tag{4.19}$$

and for the classical case a nonseparable superpotential

$$\mathcal{V}(Q_1, Q_2; q_1, q_2) = \frac{\lambda}{2}\Big(Q_1 - q_1 - (Q_2 - q_2)\Big)\Big(Q_1 + q_1 - (Q_2 + q_2)\Big)^3 \quad . \tag{4.20}$$

We see that besides terms , $\propto (Q_a - q_a)(Q_a + q_a)^3$, $a = 1, 2$, that do not entangle the variables of the subsystems, there are terms –in both superpotentials– $\propto Q_a Q_b, b \neq a$ which mix and entangle variables of both subsystems, as usual in quantum mechanics. Furthermore, a new feature in classical dynamics with (4.20) is that there are additional terms that couple Hilbert space and its dual and entangle corresponding states, for example,$\propto Q_a Q_b q_b^2, b \neq a$. This type of entanglement is decidely different from the usual quantum entanglement, in fact, since the quantum mechanical evolution is generated by a commutator it entangles bra- and ket-states separately, $\propto H_{ij}\rho_{jk} - \rho_{ij}H_{jk}$. Indeed, for a two-particle system, the evolution with an interaction of the type $\propto \widehat{H}_1 \otimes \widehat{H}_2$ has the following commutator structure

$$[\widehat{H}_{int}, \widehat{\rho}] = \widehat{H}_1\widehat{\rho}_1 \otimes \widehat{H}_2\widehat{\rho}_2 - \widehat{\rho}_1\widehat{H}_1 \otimes \widehat{\rho}_2\widehat{H}_2 \quad . \tag{4.21}$$

Again, it may be surprising that we find such terms also in classical mechanics, due to the superopotential $\mathcal{V}$ which, in the case of polynomial interactions *always* contains a contribution proportional to the usual quantum mechanical terms. However, the classical evolution produces additional correlations in $\hat{\rho}$, due to the generator $\propto \mathcal{L}_{ij;kl}\rho_{kl}$, which possibly *entangles bra- and ket-states.* In comparison with the commutator structure above, for example, such terms can have the unfamiliar structure:

$$\widehat{H_1'}\widehat{\rho}_1 \otimes \widehat{\rho}_2\widehat{H_2'} - \widehat{\rho}_1\widehat{H_1'} \otimes \widehat{H_2'}\widehat{\rho}_2 \quad , \tag{4.22}$$

which differs decidedly from a commutator. This leads us to distinguish *intra-* (i.e., within given tensor product Hilbert space of subsystems "1" and "2") and *inter-space entanglement* (i.e., between said Hilbert space and its dual).

Chapter 5

Conclusion

Aim of this thesis has been to contribute to the study of the quantum-classical divide. A central role has been played by Liouville space. Without it the interpretation of the Liouville equation in terms of the von Neumann equation, including a characteristic superoperator, would not have been found. The resulting parallel treatment makes alvaible new powerful tools for the study of differences between the classical and the quantum world.

We have seen that in the case of constant, linear, and quadratic potentials the two theories represent the same evolution and also we have learned that the von Neumann equation can describe the propagation of a free classical particle. The derived path integral and the corresponding perturbative expansion have permitted us to study the case of an anharmonic potential. We have shown analytically and graphically, that the resulting perturbative is a short time-expansion. Given an initial density matrix representing a pure plane wave state, we have propagated it for classical and quantum dynamics and after that we have delineated the region where we can trust the perturbative expansion.

We have given preliminary arguments for a new type of (dynamically assisted) entanglement (generation). The quantum evolution is generated by a commutator of the Hamiltonian with the density operator. It generally entangles underlying bra- and ket-states separately. However, the structure of the classical evolution can also entangle bra-states and ket-states simultaneously, as well as separately. In fact, polynomial interactions always contain a contribution proportional to the usual quantum terms and another decidedly classical one. Nevertheless, there is clearly a dynamical feature missing, which governs the crossing of the quantum-classical divide and it may be interesting to further investigate in this direction.

The theory can be extended in a straightforward way to the case of multi-particle systems. Last not least, the new path integral for classical dynamics will be very useful to study dynamical problems in classical statistical physics.

Appendix: The Trotter product formula

In this appendix based on Schulman's book [1], we show that the Trotter product formula for ordinary operators on Hilbert space is also valid for superoperators on Liouville space. First we define some terms that will be used

Definition: A *contraction semigroup* (for more details see [10]) on Banach space X is a family of bounded everywhere defined linear operator operators P^t, $0 \leq t < \infty$ mapping $X \to X$ such that

$$P^0 = 1 \quad , \quad P^t P^s = P^{t+s} \quad , \quad 0 \leq t, s \leq \infty \quad ,$$
$$||P^t|| \leq 1 \quad , \quad 0 \leq t < \infty \quad ,$$
$$\lim_{t \to 0} \; P^t \psi = \psi \quad \psi \in X \quad .$$

The norm used above is defined as follows:

$$||Q|| = \sup_{\psi \in X} \frac{||Q\psi||}{||\psi||} \quad ,$$

and $||\psi||$ is the norm in X. The term "contraction" comes form the fact that $||P^t|| \leq 1$, since vectors do not grow as they evolve under $||P^t||$. The *infinitesimal generator* A of P^t is defined by

$$A\psi = \lim_{t \to 0} \; \frac{1}{t}(P^t \psi - \psi) \quad , \tag{1}$$

on the domain $D(A)$ of all $\psi \in X$ for which the limit exists. Now we illustrate what we consider for Banach space X, operators P^t, Q^t, R^t, and generators A, B, $A + B$.

Our Banach space X is the Liouville space $\mathcal{L}$; it is a linear vector space as we have shown in Sect.2.4, where we have defined a scalar product and consequently a norm. Our ψ is the density vector ρ. The scalar product between two vectors is

$$\langle\langle C|D\rangle\rangle \equiv Tr(C^\dagger D) \quad . \tag{2}$$

Then, we can define a norm of a vector:

$$||D|| \equiv (\langle\langle D|D\rangle\rangle)^{\frac{1}{2}} = \left[Tr(D^\dagger D)\right]^{\frac{1}{2}} \quad . \tag{3}$$

To check that this norm is well defined, we must show that the properties of a norm are satisfied. First, we check that this norm is positive

$$Tr(D^\dagger D) = \sum_i \langle i|D^\dagger D|i\rangle = \sum_{i,j} \langle i|D^\dagger|j\rangle\langle j|D|i\rangle \quad , \tag{4}$$

$$\langle i|D^\dagger|j\rangle = \langle Di|j\rangle = (\langle j|D|i\rangle)^* = D^*_{ji} \quad ,$$

$$Tr(D^\dagger D) = \sum_{i,j} D^*_{ji} D_{ji} = \sum_{i,j} |D_{ji}|^2 > 0 \quad . \tag{5}$$

Furthermore,

$$||\lambda D|| = (\langle\langle \lambda D|\lambda D\rangle\rangle)^{\frac{1}{2}} \left[Tr(\lambda^* D^\dagger \lambda D)\right]^{\frac{1}{2}} = |\lambda| \; ||D|| \quad , \tag{6}$$

and finally, without proof but we state that as a consequence of the scalar product being positive semi-definite and by the previuos definition of the norm, we have the triangle inequality

$$||C + D|| \leq ||C|| + ||D|| \quad . \tag{7}$$

Now that we have a norm for vectors in Liouville space, we define a norm of a superoperator in a completely analogous way to the norm on Banach space

$$||\mathcal{H}|| = \sup_{\rho\in\mathcal{L}} \frac{||\mathcal{H}\rho||}{||\rho||} = \sup_{\rho\in\mathcal{L}} \left(\frac{\mathrm{Tr}(\rho^\dagger \mathcal{H}^\dagger \mathcal{H}\rho)}{\mathrm{Tr}(\rho^\dagger\rho)}\right)^{\frac{1}{2}} \quad , \tag{8}$$

For the physical interpretation, we identify the operators and the generators:

$$P^t = e^{-i\mathcal{T}t}, \quad Q^t = e^{-i\mathcal{V}t}, \quad R^t = e^{-i\mathcal{H}t} \quad . \tag{9}$$

If we use the definition of generator (1) we obtain:

$$A = -i\mathcal{T}, \quad B = -i\mathcal{V}, \quad A + B = -i\mathcal{H} \quad . \tag{10}$$

However, we still have to check that these operator satisfy the properties required for a contraction semigroup. The only non-trivial property is the boundeness of the operators.

For Q^t, there is no problem, since $\mathcal{V}$ is a diagonal, real, multiplicatively acting super-operator. Indeed,

$$\begin{aligned} ||e^{-i\mathcal{V}t}\rho||^2 = \mathrm{Tr}\left[\rho^\dagger e^{i\mathcal{V}^\dagger t} e^{-i\mathcal{V}t}\rho\right] = \mathrm{Tr}\left[\rho^\dagger e^{i\mathcal{V}t} e^{-i\mathcal{V}t}\rho\right] &= \mathrm{Tr}\left[\rho^\dagger \rho\right] && (11) \\ &= \mathrm{Tr}\left[\rho^2\right] && (12) \\ &\leq \mathrm{Tr}\left[\rho\right] = 1 \quad , \end{aligned}$$

for a normalized density matrix. Then

$$||e^{-i\mathcal{V}t}\rho|| \leq 1 \quad , \tag{13}$$

for all t. For P^t, we review some elementary facts about the norm. Generally speaking, the norm looks for the largest eigenvalue. If X is finite (M) dimensional, we have $Q\psi_i = q_i\psi_i$, $i = 1, ..., M$. Then, the worst case is the biggest $|q_i|$, call it $|\overline{q}|$ and its eigenvector $\overline{\psi}$; then, $||Q|| = \max_\psi ||Q\psi||/||\psi|| = ||Q\overline{\psi}||/||\overline{\psi}|| = |\overline{q}|$. Let $Q = e^C$, its eigenvalues are e^{C_i}, where C_i are the eigenvalues of C. Then $||e^C|| = \max_i \ |e^{C_i}| = \max_i \ |e^{Re \ C_i}|$. Thus,

$$||e^{tC}|| = \max_i \ e^{t\mathrm{Re} \ C_i} \quad , \tag{14}$$

so that the condition for C to be the generator of a contractive semigroup is that Re $C_i \leq 0$, for all i. On Banach space, the object that would be the eigenvector is not always in the space and the definition of the norm as a limit ("sup") must be invoked. We must use the definition of the spectrum, which is defined as the complement of the resolvent set, where the resolvent set of an operator Q is the set of all λ for which $(\lambda - Q)^{-1}$ exists. Above we had a condition on the eigenvalues of a finite dimensional matrix C so that a contractive semigroup is generated. In a Banach space, it is most convenient to state the condition in terms of the spectrum. Thus condition for an operator C is that Re$\lambda \leq 0$, for λ in the spectrum. If $C = iK$, in terms of the eigenvalues (or spectrum) k_i of K this means Im$k_i \geq 0$, for all i. If e^{-tC} also is to be a contractive semigroup-evolution in both directions we must have

$$\mathrm{Im} \ k = 0 \quad .$$

That is, K has only a real spectrum, a condition guaranteed by the usual requirement that the Hamiltonian be self-adjoint. In order to determine whether $A + B$ generate a contractive semigroup, we examine whether $\mathcal{T} + \mathcal{V}$ is self-adjoint (so that its spectrum is real), if this is true, then all conditions for the Trotter formula are satisfied.

Consequently, we arrive at the theorem used in Sect. 2, 2.5.

THEOREM: (Trotter formula) Let A and B be linear operators on a Banach space X, such that A, B, and $A + B$ are the infinitesimal generators of a contraction semigroup P^t, Q^t, and R^t, respectively. Then for all $\psi \in X$

$$R^t\psi = \lim_{n\to\infty} (P^{\frac{t}{n}} Q^{\frac{t}{n}})^n \psi \quad . \tag{15}$$

In this way, our Feynman path integral for classical dynamics is justified by the foregoing theorem, where by sum over histories is meant the specific way of doing this sum which amounts to taking the n-th power of a finite operator (for standard detailed proofs of the theorem see [5],[10],) .

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