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Introduction des frottements pour un système
dissipatif quantique évoluant dans le temps

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بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

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الْأَكْرَمُ ۝٣ الَّذِي عَلَّمَ بِالْقَلَمِ ۝٤ عَلَّمَ الْإِنْسَانَ مَا لَمْ يَعْلَمْ ۝٥

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Introduction

To study any physical system, it is important to find firstly a simple framework where the most important parameters are expressed and analyzed. However, realistic situations are far from being that simple as plenty of uncontrolled factors enter into play and the system becomes unavoidably more complex. This is clearly the case when considering dissipation or friction in the evolution of any physical system. Indeed, dissipation is an important player to consider in the dynamical study as it affects the energy hence annihilating the most important rule in physics which is the energy conservation rule.

Studying dissipation in the framework of classical physics is a tedious task as it resorts to phenomenal considerations that break for the most the simple Lagrangian description. The task becomes even more complex when studying dissipation for quantal systems since the correspondence classical-quantal for dissipative systems is less obvious. We are left then with few guidelines in order to reproduce physical behavior.

This master project is an attempt to shed light on the main difficulties we encounter when tackling quantal dissipative systems. For this we are studying the evolution in time of a Gaussian wave packet as it impinges on a square barrier potential with damping profile. In the non-dissipative regime and with the appropriate conditions this will lead to the standard tunnel effect where a fraction of the wavepacket is transmitted through the barrier. We are interested in illustrating how the transmission is affected by the friction. The dissipation contribution is treated in the framework of the Caldirola-Kanai model and a FORTRAN program is built for the numerical implementation. The evaluation is performed in order to lead to conclusive results.

This master thesis is organized in three chapters:

- The first chapter is a brief review of the physics of the non-dissipative systems at the classical and quantal level. It presents also the formalism behind the use of the wave packet describing the state of the system. It terminates with the presentation of a practical and analytical case of the free wave packet evolution.

- The second chapter is a brief review of the dissipative systems. It aims at presenting the most important models that are devised in order to incorporate dissipation in the description of the system. We are giving in this review some of the problems that arise when a quantal

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correspondence is desired. Here also we are terminating with the practical and analytical case of the free wave packet evolving in a medium with a constant friction factor

-In the last chapter we are presenting the main numerical aspects of the problem and strategy for translating these aspects in a FORTRAN program. The validation of this program is done through a comparison of the numerical results to the results found for the analytical cases cited above. The results for the realistic case of the square barrier with a friction profile are then exposed and the most important features are highlighted.

CHAPTER I: CONSERVATIVE SYSTEMS

I. Introduction

In our attempt to study nonconservative systems in the framework of the evolution of a gaussian wave packet submitted to frictions, we should first review some of the most important features and theory related to conservative systems. This is important in order to understand the transition between the two types of systems but also in order to be able to establish comparison that allows the appreciation of the effectiveness of some adopted models for friction. We recall in this review some of the theory for classical as well as quantal systems. As we know even if we are interested in quantal systems, the evolution of the mean value is still classical as clearly stipulated by the Ehrenfest theorem.

A. Classical conservative systems

Rather than just giving the final Newton equation that governs the classical evolution of the coordinates, let us start from a more fundamental point of view which is the concept of the action and the principle of least action or more accurately the stationary action. Doing so, the formulation of any dynamical problem become free of the choice of the coordinate system and is only related to the evolution of its energy.

I. Action and principle of least action

For each physical system, there is a quantity which is the system's action. It depends on the way the system evolves. In other words, the action is an attribute of the dynamics of a physical system. It is a mathematical functional which takes the trajectory, also called path or history of the system as its argument and has a real number as its result. Generally, the action takes different values for different paths. Action has the dimensions of [energy]·[time], and its SI unit is joule-second. This is the same unit as that of angular momentum. The action is typically represented as an integral over time, taken along the path of the system between the initial time and the final time (figure.I.1) of the evolution of the system:

$$A = \int_a^b L dt \quad (1.1)$$

Where the integrand L , is called the Lagrangian of the system. The Lagrangian is given as the difference between the kinetic and the potential energies. For the action integral to be well-defined the trajectory has to be bounded in time and space.



Fig.I.1 For the different paths between the initial position A and the final position B, only the one with the extremum action will be the true one

The principle of least action (PLA) or rather a stationary action is the principle that stipulates that a system's actual evolution is such that the system has a quantity of action that is an extremum relative to other quantities of action for the other paths. Given the PLA, and once the action of a system has been formulated, we can deduce its equations of motion.

The least action principle stipulates that the action of a motion between two-point "a" and "b" in the configuration space defined by the time integral $A = \int_a^b L dt$ on a given path from "a" to "b" must be a stationary on the unique true path for a given period of time t of the motion between the two points:

$$\delta A = \delta \int_a^b L dt = 0 \quad (1.2)$$

This principle yields the famous Lagrange-Euler equation given by:

$$\frac{\partial}{\partial t} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \quad (1.3)$$

Where $\dot{q} = \frac{\partial q_i}{\partial t}$. These above equations underline a completely deterministic dynamic process: if the time period of the motion is given, there is only one path between two given points so that all the states of the systems are completely determined by equation (1.3) for every moment of the motion. However, this deterministic character of the dynamics does not exist anymore when the motion becomes random and stochastic. [1][2]

II. The Lagrangian formalism

The Lagrangian formalism is the use of Hamilton's principle of stationary action or the principle of least action for the derivation of the equations of motion of a system. Let us start

with an N-particle system in which the forces can be derived from a potential function $V(x)$. We shall denote the x, y and z coordinates of all the particles by the general letter x , giving it an index where necessary: $x_i, x = 1, \dots, n$. The system's kinetic energy can be written in the form: $T = \frac{1}{2} \sum_i m_i \dot{x}_i^2$

and with this we define the Lagrangian function:

$$L = (x, \dot{x}) = T(\dot{x}) - V(x) \quad (1.4)$$

This is resembling the energy except for a change in sign. Newton's equations of motion can now be written as:

$$\frac{\partial L}{\partial x_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i} = 0 \quad (1.5)$$

Which we abbreviate as:

$$\frac{\partial L}{\partial x_i} = 0 \quad (1.6)$$

Two facts can be deduced from this formula. The first is that L can be used in a variational formulation of the laws of motion that will be closely analogous to Fermat's principle in optics. The second important fact about equation (1.6) is that it can immediately be generalized to other kinds of coordinates.

The remarkable feature of Lagrange's equations that is now to be proved is that if we write: $x_i = x_i(q_i, \dots, q_n)$ or $x(q)$ for short, the functional derivative of L with respect to q becomes:

$$\frac{\partial L}{\partial q_n} = \sum_{i=1} \frac{\partial L}{\partial x_i} \frac{\partial x_i}{\partial q_n} \quad (1.7)$$

so that from equation (1.6) we can conclude that the laws of motion take exactly the same form

in generalized coordinates: $\frac{\partial L(q, \dot{q})}{\partial q_n} = 0$

we can write: $\frac{\partial L}{\partial q_n} = \frac{\partial L}{\partial x_i} \frac{\partial x_i}{\partial q_n}$

To change variable, we have: $\frac{\partial L}{\partial q_n} = \frac{\partial L}{\partial q_n} \frac{\partial x_i}{\partial q_n} + \frac{\partial L}{\partial \dot{x}_i} \frac{\partial \dot{x}_i}{\partial q_n}$

Since x_i does not depend on \dot{q} , we have next:

$$\frac{\partial L}{\partial \dot{q}_n} = \frac{\partial L}{\partial \dot{x}_i} \frac{\partial \dot{x}_i}{\partial \dot{q}_n} \quad (1.8)$$

Finally, we can write:

$$\frac{\partial L}{\partial q_n} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_n} = 0 \quad (1.9)$$

These are the required Lagrange's equations of motion derived from the Hamilton's stationary principle. The equation also shows that the Lagrange's equations of motion for holonomic system are necessary and sufficient conditions for action to have a stationary value.[4/5/6]

III. The Hamiltonian Formulation

By performing a Legendre transformation of the Lagrangian, we can establish what is known in classical mechanics as the Hamiltonian. It is defined as a function of the canonical coordinates and momenta which satisfies Hamilton's principle:

$$\delta \int_a^b \{ \sum_{i=1}^k \dot{q}_i p_i - H(p_i, q_i) \} dt = 0 \quad (1.10)$$

Where q_i is the coordinates, p_i the momentum, H the Hamiltonian given by:

$H = T + V$, T is the kinetic energy, V is the potential energy and k the number of degrees of freedom of the system.

This integral between any two arbitrary times a and b for the actual path must be minimum (or extremum). This requirement gives us Hamilton's canonical equations:

$$\dot{q}_i = \frac{\partial H(p_i, q_i)}{\partial p_i} \quad \dot{p}_i = - \frac{\partial H(p_i, q_i)}{\partial q_i}, \quad i = 1, \dots, n \quad (1.11)$$

These first order differential equations for $q_i(t)$ and $p_i(t)$ determine the position and momentum of the i^{th} degree of freedom as a function of time if we assume that the initial conditions are known:

$$q_i(t = 0) = q_0(0), \quad p_i(t = 0) = p_0(0) \quad (1.12)$$

By eliminating p_i between the two sets of equation (1.11), we find the Newton equations of motion:[3][4][5]

$$m_i \ddot{q}_i = F_i(q_1, \dots, q_n, \frac{\partial H}{\partial p_1}, \dots, \frac{\partial H}{\partial p_n}) \quad (1.13)$$

IV. Newton's law of motion and equations of motion:

We recall here the more familiar law of motion of Newton that can be derived in a more general way from the Euler-Lagrange equation or the Hamilton equations. The motion of a particle is governed by Newton's second law, relating the unbalanced forces on a particle to its acceleration. If more than one force acts on the particle, the equation of motion can be written:

$$\sum F = F_R = ma$$

$$m\ddot{x} + kx = 0 \quad (1.14)$$

Where $F_R = -kx$ is the resultant force, which is a vector that sum all the forces. Here, we assume that the force is the gradient of the quadratic potential. [1][7]

B. Quantum conservative systems

The principal object of classical dynamics is to find where every thing is at time t ; that is, to find a set of $q_n(t)$. The principal object of quantum mechanics is to find a wave function $\psi(q, t)$. From this we cannot calculate where every thing is in the sense of classical physics, but you can calculate all there is to know. The Lagrangian and Hamiltonian dynamics find $q(t)$ and $\dot{q}(t)$ or $p(t)$ by means of ordinary differential equations. In $\psi(q, t)$, q is in no sense a function of t , since ψ has a value for every q and every t . The equation it solves is a partial differential equation. The differences between the two mathematical descriptions are so wide that they seem to belong to different universes of ideas. It is worth mentioning at this level that the quantum mechanics is a theory built on a set of mathematical postulates but a century after its birth, none of these postulates revealed to be wrong.

We are going in this section recall some of the most important fundamentals of quantum physics. Encompassing all the aspects of the field in the scope of this thesis is out of reach consequently we are going to focus on the concepts which we are going to use in developing our problematic.

I. Brief review of quantum physics basics

I.1. The wave function

As we have stated just above the state of the quantal system is no longer given in terms of the relationship between the generalized coordinate versus the time but are rather given by a value at each time and space position otherwise in terms of a wave function $\psi(q, t)$. Besides being a mathematical function, which has no physical meaning, the square of the modulus of this function $|\psi(q, t)|^2$ expresses the density probability of finding the particle at the position “ q ” and at the time “ t ”.

I.2. The operational representation

Associated with each measurable parameter in a physical system is a quantum mechanical operator. The application of this operator to the state of the system gives the eigen values that can be associated within a certain probability to the physical measure. For these eigen values to be real, the operator must be Hermitian.

The operator associated with the system energy is called the Hamiltonian. In classical mechanics, the system energy can be expressed as the sum of the kinetic and potential energies. For quantum mechanics, the elements of this energy expression are transformed into the corresponding quantum mechanical operators. The Hamiltonian contains the operations associated with the kinetic and potential energies and for a particle in one dimension can be written:

$$H = \frac{p^2}{2m} + V(x) \quad (1.15)$$

And $p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$, the equation (1.15) becomes:

$$H = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (1.16)$$

The expectation or the mean value of any measurable quantity α is given by the mean value of the operator $\hat{\alpha}$ representing the quantity as:

$$\langle \hat{\alpha} \rangle = \langle \psi^* | \hat{\alpha} | \psi \rangle = \int d\vec{r} \psi^* \hat{\alpha} \psi \quad (1.17)$$

I.3. Schrodinger equation

The central part in the study of any quantum system is the determination of the wave function that will contain all the information we want to know about the system. A way to reach this function is to solve the Schrodinger equation. It is a differential equation that will govern the evolution the system according to its Hamiltonian.

Consider for example a particle of mass m moving in a one-dimensional space x under the influence of a potential $V(x, t)$, the time-dependent Schrodinger equation is given by:

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \left[\frac{p^2}{2m} + V(x, t) \right] \psi(x, t) \quad (1.18)$$

This equation is analytically solvable only for simple cases ($V(x) = 0$ or simple forms of $V(x)$), otherwise this equation is very complex and most of the time we will be using numerical recipes to try to be as close as possible to the physical solution.

I.4. Ehrenfest theorem

Ehrenfest's theorem simply states that expectation values of quantum mechanical operators obey the laws of classical mechanics. In general terms, the time variation of expectation value of any arbitrary quantum mechanical operators given by:

$$\begin{aligned} \frac{d\langle \alpha \rangle}{dt} &= \frac{d}{dt} \int d\vec{r} \psi^* \hat{\alpha} \psi \\ &= \int d\vec{r} \left[\frac{\partial \psi^*}{\partial t} \alpha \psi + \psi^* \frac{\partial \alpha}{\partial t} \psi + \psi^* \alpha \frac{\partial \psi}{\partial t} \right] \\ &= \left\langle \frac{\partial \alpha}{\partial t} \right\rangle + \frac{1}{i\hbar} \int d\vec{r} \left[- \left(-i\hbar \frac{\partial \psi^*}{\partial t} \right) \alpha \psi + \psi^* \alpha \left(i\hbar \frac{\partial \psi}{\partial t} \right) \right] \end{aligned} \quad (1.19)$$

Making use of time-dependent Schrodinger equation (1.18), and its complex counterpart, we arrive at:

$$\begin{aligned} \frac{d\langle \alpha \rangle}{dt} &= \left\langle \frac{\partial \alpha}{\partial t} \right\rangle + \frac{1}{i\hbar} \int d\vec{r} \psi^* (\alpha \hat{H} - \hat{H} \alpha) \psi \\ \frac{d\langle \alpha \rangle}{dt} &= \left\langle \frac{\partial \alpha}{\partial t} \right\rangle + \frac{1}{i\hbar} \langle [\alpha, \hat{H}] \rangle \end{aligned} \quad (1.20)$$

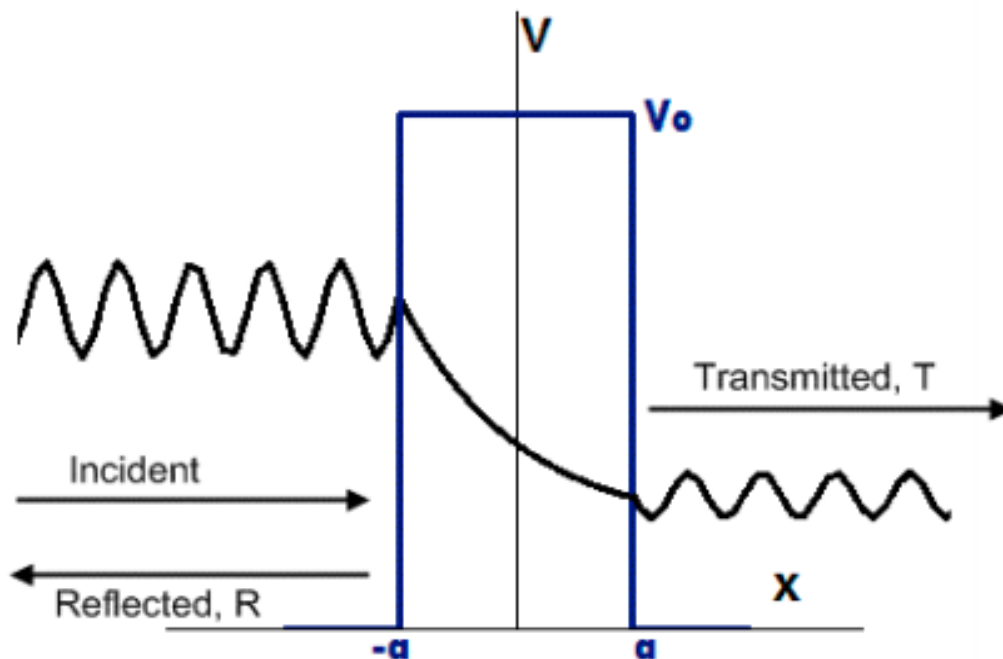
Where the commutator $[\alpha, \hat{H}]$ is equal to $\alpha \hat{H} - \hat{H} \alpha$. If this amount equation (1.20) is equal to zero we say that α is a constant of motion. [8][9]

I.5. Tunnel effect

Quantum tunnelling is the quantum mechanical phenomenon where a wave function can propagate through a potential barrier even if the energy of the particle is less than the height of the barrier. The transmission through the barrier can be finite and depends exponentially on the barrier height and barrier width. The wave function may disappear on one side and reappear on the other side. The wave function and its first derivative are continuous. In steady-state, the probability flux in the forward direction is spatially uniform. No particle or wave is lost (figureI.2).

We are recalling in this section briefly the notion of quantum tunneling, since we are interested in our study to see how the tunneling properties are affected by the friction factor. The most important parameter that is affected by the friction is the transmission coefficient which is the fraction of the wave that penetrates the barrier and could be given as: [10]

$$T_{wp}(E_i) = \int_0^{+\infty} dq |\psi(q, t_f, E_i)|^2 \quad (1.21)$$



FigI.2. Tunneling of a wave function through a rectangular barrier

II. The gaussian wave packet evolution

II.1. Wave or wave packet?

To introduce quantum mechanics, we always talk about a wave function as representing the particle state. From otherside we do know that the Schrodinger equation solution for a free particle is a plane wave (a sine function) that extends in the whole space. This comes as a natural consequence of the Heinsberg indetermination principle. Indeed, assuming in this case that the momenta of the particle is precisely determined ($\Delta p = 0$) implies that $\Delta x = 0$. We say that the particle is delocalized. This comes as a counter sense since we know that the particle is some where. The only way to circumvent this problem is to allow some uncertainty on the momenta P (or equivalently the wave vector k), this means that we are superposing a number of sine functions that lead to the creation of the wave packet (figure I.3). Actually, the wave packet is a way to reconcile the corpuscle and wave natures of the quantum particles.

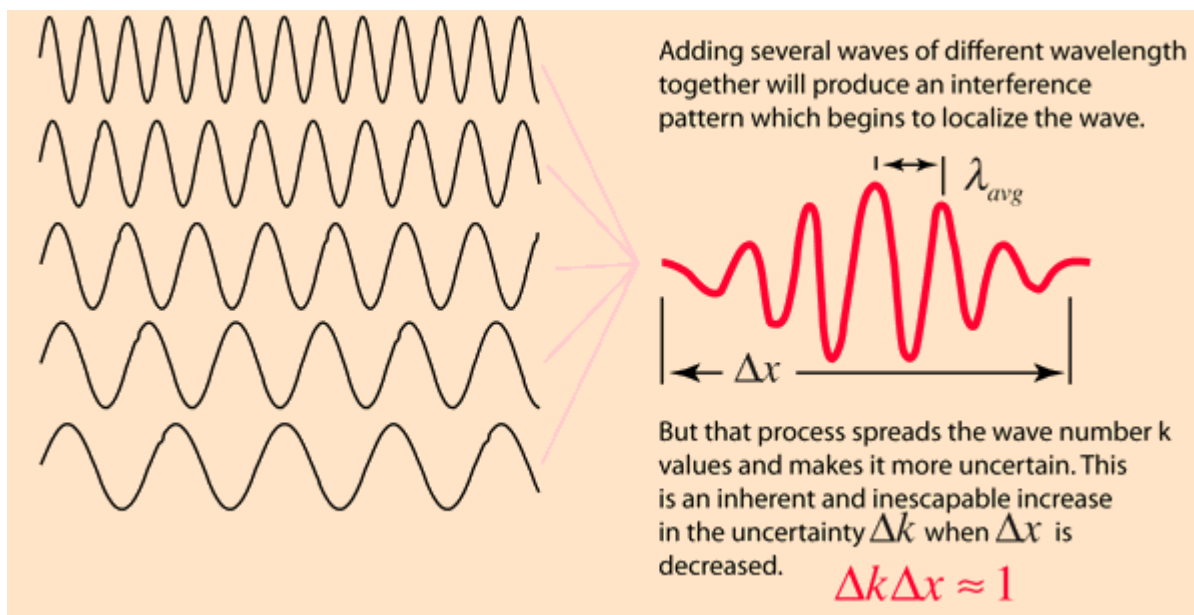


Fig.I.3. Construction of the wave packet from sine functions

II.2. Profile of the Gaussian wave packet

The superposition of an infinite number of plane waves of different wave number, needed to localize a particle, can be achieved through the formula:

$$\psi(x, t) = \int_{-\infty}^{+\infty} \bar{\psi}(k) e^{i(kx - \omega t)} dk \quad (1.22)$$

Using the Fourier's theorem, which states that if:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \bar{f}(k) e^{ikx} dk \quad (1.23)$$

then:

$$\bar{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx \quad (1.24)$$

Here, $\bar{f}(x)$ is known as the Fourier transform of the function $f(x)$. We can use Fourier transform to find the k space function $\bar{\psi}(k)$ which generates any given x space wave function $\psi(x)$ at a given time.

Suppose that at $t = 0$, the wave function of our particle takes the form of a Gaussian then:

$$\psi(x, 0) \propto \exp \left[ik_0 x - \frac{(x-x_0)^2}{4(\sigma)^2} \right] \quad (1.25)$$

Where x_0 is the mean value, and sigma is the variance of the Gaussian where and the amplitude has yet to be determined to normalize this function.

Thus, the initial probability density of the particle is written:

$$|\psi(x, 0)|^2 \propto \exp \left[-\frac{(x-x_0)^2}{2(\sigma)^2} \right] \quad (1.26)$$

This particular probability distribution is called a Gaussian distribution, and is plotted in (figure I.4). It can be seen that a measurement of the particle's position is most likely to yield the value x_0 , and very unlikely to yield a value which differs from x_0 by more than $3\Delta x$. Thus, the equation (I.26) is the wave function of a particle which is initially localized around $x = x_0$ in some region whose width is of order Δx . This type of wavefunction is known as a Gaussian wave packet.

Now, according to equation (I.22)

$$\psi(x, 0) = \int_{-\infty}^{+\infty} \bar{\psi}(k) e^{ikx} dk \quad (1.27)$$

Hence, we can employ Fourier's theorem to invert this expression to give:

$$\bar{\psi}(k) \propto \int_{-\infty}^{+\infty} \psi(x, 0) e^{-ikx} dx \quad (1.28)$$

An elementary and well known equation (1.27) analysis based on completing squares in the exponent of the integrals gives then: [11]

$$\bar{\psi}(k) \propto \exp \left[-ikx_0 - \frac{(x-x_0)^2}{4(\Delta k)^2} \right] \quad (1.29)$$

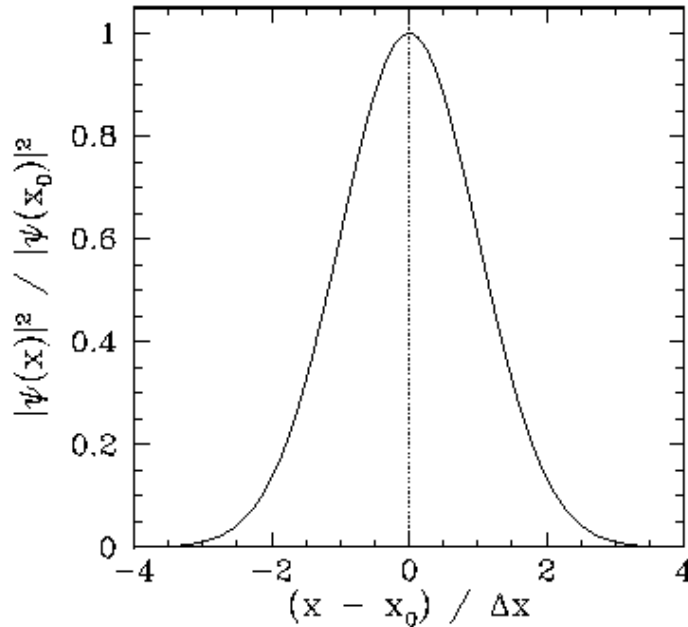


Fig I.4. A gaussian wave packet with the most important parameters

Where:
$$\Delta k = \frac{1}{2\sigma}$$

Now, if $|\psi(x)|^2$ is proportional to the probability density of a measurement of the particle's position yielding the value x then it stands to reason that $|\bar{\psi}(k)|^2$ is proportional to the probability density of a measurement of the particle's wave number yielding the value k (Recall that $p = \hbar k$, so a measurement of the particle's wave number k is equivalent to a measurement of the particle's momentum p). According to equation (1.28):

$$|\bar{\psi}(k)|^2 \propto \exp \left[-\frac{(k-k_0)^2}{2(\Delta k)^2} \right] \quad (1.30)$$

Note that this probability distribution is a Gaussian in k space. Hence, a measurement of k is most likely to yield the value k_0 , and very unlikely to yield a value which differs from k_0 by more than $3\Delta k$. Incidentally, a Gaussian is the only mathematical function in x space which has the same form as its Fourier transform in k space.

We have just seen that a Gaussian probability distribution of characteristic width Δx in x space transforms to a Gaussian probability distribution of characteristic width Δk in k space, where:

$$\sigma \cdot \Delta k = \frac{1}{2}$$

This illustrates an important property of wave packets. Namely, if we wish to construct a packet which is very localized in x space (i.e., if Δx is small) then we need to combine plane waves with a very wide range of different k values (i.e., Δk will be large). Conversely, if we only combine plane waves whose wave numbers differ by a small amount (i.e., if Δk is small) then the resulting wave packet will be very extended in x space (i.e., σ will be large).

To finish this section, we recall that if a motion of the wave packet is considered then we have to deal with two types of velocity:

-The group velocity which is the speed of the centroid or the mean value of the packet position that can be established by the Ehrenfest relation. This speed amount has a classical behavior.

-And a phase speed and this is related the nodes speed or the speed of waves composing the packet and can be given by the relation:

$$V_p = \frac{d\omega}{dk}$$

ω being the angular frequency and k the wave vector. [11][12]

II.3. Motion of wave packet without dissipation:

Once we have introduced all the ingredients, let us consider the evolution in time of a free Gaussian wave packet, moving with no dissipation. We shall be looking for wave function $\psi(x, t)$ satisfying the free time dependent Schrödinger equation and having a definite form $f(x)$ at $t = 0$, that is:

$$i \frac{\partial \psi}{\partial t} = -\frac{1}{2} \frac{\partial^2}{\partial x^2}$$

$$\psi(x, 0) = f(x) \quad (1.31)$$

Where here we are working in natural units: the masse of the particle $m = \hbar = 1$

Using Fourier integrals $\psi(x, t)$ can be expressed as:

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(p) \exp [i (px - \frac{1}{2} p^2 t)] dp \quad (1.32)$$

$$g(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ipx} f(x) dx \quad (1.33)$$

We shall assume $f(x)$ having a gaussian form:

$$f(x) = \frac{1}{\sqrt{\sigma\pi^{\frac{1}{4}}}} e^{-\frac{(x-x_0)^2}{2\sigma^2}} e^{ip_0x} \quad (1.34)$$

So that $|f(x)|^2$ is normalized and gives a probability density concentrated around x_0 with a dispersion $\Delta x = \sigma$.

As we have seen before the Fourier transform in this case is given by:

$$g(p) = \frac{\sqrt{\sigma}}{\pi^{\frac{1}{4}}} e^{-i(p-p_0)x_0} e^{-\frac{\sigma^2(p-p_0)^2}{2}} \quad (1.35)$$

And then we have:

$$\psi(x, t) = \frac{\sqrt{\sigma}}{\pi^{\frac{1}{4}}\sqrt{\sigma^2+it}} e^{i(p_0x-\frac{1}{2}p_0^2t)} e^{-\frac{(x-x_0-p_0t)^2}{2(\sigma^2+it)}} \quad (1.36)$$

The probability density for finding the particle at the point x at time t is then given by:

$$p(x, t) \equiv |\psi(x, t)|^2 = \frac{1}{\sqrt{\pi}\sigma\sqrt{(1+\frac{t^2}{\sigma^4})}} \exp\left\{-\frac{(x-x_0-p_0t)^2}{\sigma^2(1+\frac{t^2}{\sigma^4})}\right\} \quad (1.37)$$

Clearly at time t the center of the wave packet has moved from $x = x_0$ to $x = x_0 + p_0t$, i.e., it moves with group velocity p_0 . The width of the wave packet also changes from σ to $\sigma[1 + (\frac{t^2}{\sigma^4})]^{\frac{1}{2}}$ quantifying the natural spreading which is the result of the difference between the phase velocity of the modes composing the wave packet (see figure I.5). [12]

This analytical result possible only for a free Gaussian wave packet, will be considered as benchmark to test the validity of our coded software. An analytical result is also possible for the case of a constant friction in the whole space as will be seen in chapter two. These two analytical results will be the starting point for our comparison and for a more extended investigation.

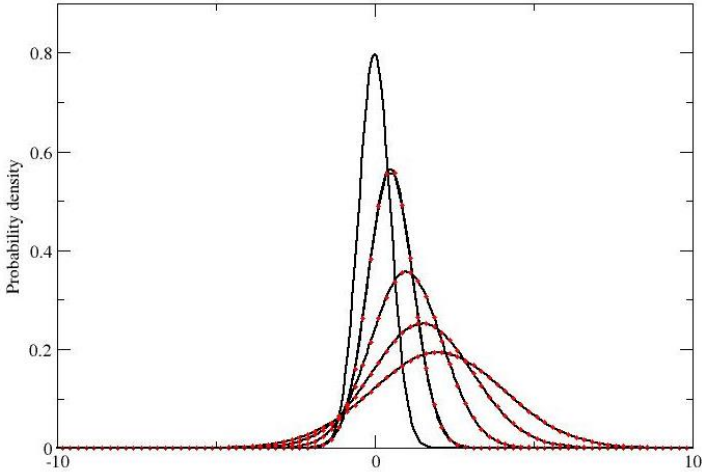


Fig I.5. Spreading of the free wave packet as it evolves in time

CHAPTER II: NON CONSERVATIVE SYSTEMS

I. Introduction

The main scope of this study is to feature basically open quantum systems or in other words non conservative systems. In the first chapter we have addressed a basic review of the main tools needed to study conservative systems at the classical and quantal levels. A practical case of calculation of the motion of a quantal Gaussian wave packet was presented. Is it possible to extend the same formalism to the case of non conservative systems by establishing a way that introduces the friction felt by the system? It will be seen that the case of non conservative systems is not obvious neither for classical nor for quantal systems. This will explain the recourse to phenomenological approaches where the only guideline is to reproduce the equation of motion for these systems.

In this second chapter we will present a brief review of some of the phenomenological approaches that are used for the classical systems. We will see how the canonical relations are used to extend these formulations to quantal systems. We will see also that a similar equation of motion is adopted in average for a quantal system with different modulizations of the dissipation occurring during the system motion. For the quantal treatment we will distinguish two approaches: the semi quantal (or phenomenological) treatment where the dissipation is introduced in a phenomenological way as the Caldirola-Kanai and Kostin-Albrecht method and the pure microscopic approach as given by the Caldeira-Legett method. To integrate a more general type of dissipations which are of stochastic nature, the stochastic Langevin equation as phenomenological approach to classical systems, is introduced. Finally, to illustrate the case of non conservative systems, we present the analytical case of the motion of a Gaussian wave packet in a medium with a constant rate of friction.

II. Classical non conservative systems

II.1. The Lagrangian formalism

As we have seen in the previous chapter the description of any classical systems begins with the definition of its Lagrangian (or equivalently its Hamiltonian). Unfortunately, not all mechanical systems have an Euler-Lagrangian description. Couplings of a system to other degrees (environmental degrees of freedom) lead to dissipation when the number of the degrees is large and hence the energy conservation where the Lagrangian formalism is obvious is no

longer guaranteed. For example, the equations of motion for the damped oscillator are only a small modification of those of the harmonic oscillator:

$$m\ddot{q} = -kq - \gamma\dot{q} \quad (2.1)$$

but the additional force, where γ is the damping rate:

$$f = -\gamma\dot{q}$$

is not conservative.

It is not possible to add an extra potential to the Lagrangian, not even one that depends on velocities, to account for the force f . The equations of motion become of the (general) form:

$$\frac{d}{dt} \left(\frac{dL}{d\dot{q}} \right) - \frac{dL}{dq} = f \quad (2.2)$$

We can write: $f = \frac{\partial D}{\partial \dot{q}}$ with $D(\dot{q}, q) = -\frac{1}{2}\gamma\dot{q}^2$. The equation of motion becomes: [4/5/6/13]

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = \frac{\partial D}{\partial \dot{q}} \quad (2.3)$$

II.2. Caldirola-Kanai phenomenological approach

There are different strategies to construct Hamiltonian functions to account for dissipative systems and then, from them, to obtain the corresponding quantum Hamiltonian operator. One of them consists in considering time-dependent Lagrangian (and therefore Hamiltonians), which avoids us to deal explicitly with the environmental degrees of freedom. This approach preserves the canonical formalism and can be a good starting point to find out the quantal analog of the corresponding dissipative dynamics. Here, the Caldirola-Kanai Hamiltonian model constitutes a paradigm of dissipation. This model arises from the classical equation of motion for a damped particle of mass m under the action of an external potential $V(x)$. For one-dimensional models and a mean friction γ we have:

$$m\ddot{x} + m\gamma\dot{x} + \partial_x V(x) = 0 \quad (2.4)$$

with the short-hand notation $\dot{x} = dx/dt$ and $\ddot{x} = d^2x/dt^2$ for total time derivatives, and $\partial k_\eta = \partial^k / \partial \eta_k$ and for the k -th derivative with respect to a given variable η . Multiplying this equation by $e^{\gamma t}$, it can be recast as:

$$\frac{d}{dt} (me^{\gamma t}\dot{x}) + \partial_x [V(x)e^{\gamma t}] = 0 \quad (2.5)$$

If we consider the change of variable $X = x$ and:

$$P \equiv me^{\gamma t} \dot{x} = pe^{\gamma t} \quad (2.6)$$

Where $p = m\dot{x}$ is the physical momentum, we readily notice that it is just the Lagrange equation satisfied by the time-dependent Lagrangian function:

$$L = \left[\frac{1}{2} m \dot{X}^2 - V(X) \right] e^{\gamma t} = \frac{P^2}{2m} e^{-\gamma t} - V(X) e^{\gamma t} \quad (2.7)$$

where P plays the role of a canonical momentum, i.e., $P = \partial_x L$. This equation allows us by using the Legendre transformation, to obtain straight forwardly the corresponding Hamiltonian

$$H = \dot{X}P - L = \frac{P^2}{2m} e^{-\gamma t} + V(X) e^{\gamma t} \quad (2.8)$$

Which is a function of the canonical variables X and P , satisfying the Hamilton equations:

$$\dot{X} = \partial_P H, \quad \dot{P} = -\partial_X H \quad (2.9)$$

respectively. equation (2.8) defines the Caldirola-Kanai Hamiltonian. In terms of this time dependent Hamiltonian model, the system classical energy can be recast as:

$$E = \frac{p^2}{2m} + V(x) = He^{-\gamma t} \quad (2.10)$$

Which explicitly exhibits the typical exponential decay associated with equation (2.8) regardless of the implicit time-dependence that H might display [15].

In this section we shall systematically use X and P as we shall mention later that they are related to x, p by a non-canonical transformation. Apparently, the Hamiltonian is depending on t , however, it does not generally represent dissipative systems but it does represent physical systems with an exponentially increasing mass with time $m(t) = me^{\gamma t}$.

Using Hamilton's equations, we get from H that:

$$\dot{X} = \frac{\partial H}{\partial P} = e^{-\gamma t} P \quad (2.11)$$

$$\dot{P} = -\frac{\partial H}{\partial X} = -e^{\gamma t} \frac{\partial V(X)}{\partial X} \quad (2.12)$$

And thus, from equation (2.11) we have:

$$P = e^{\gamma t} \dot{X}, \quad \dot{P} = \gamma e^{\gamma t} \dot{X} + e^{\gamma t} \ddot{X} \quad (2.13)$$

Subtracting equation (2.12) from the \dot{P} in equation (2.13) and canceling the common factor $e^{\gamma t}$ we get then the equation of motion:

$$\ddot{X} + \gamma\dot{X} + \frac{\partial V}{\partial X} = 0 \quad (2.14)$$

Which is exactly the one in equation (2.14) but in terms of the X and P coordinates.

Note that in the units ($\hbar = m = 1$), we have in the non-dissipative case $p = \dot{x}$ while in equation (2.13) $P = e^{\gamma t} \dot{X}$. This implies that $P = e^{\gamma t} p$ which will be relevant for the later analysis.

II.3. Stochastic Langevin equation

Actually, the dissipation in general is not just the result of an opposition to the dynamical evolution of the system (where the friction force is proportional to the velocity and opposes the motion) but also results from a stochastic process known as a Brownian motion. In this case the equation of motion is rather well sketched by the Langevin equation.

Langevin equation (named after Paul Langevin) is a stochastic differential equation describing the time evolution of a subset of the degrees of freedom. If we consider for simplicity an open system with a single degree of freedom, which we associate with the coordinate $q(t)$ of a particle with mass m , the simplest assumptions about the dissipative process one can make is that dissipation is state independent. Then the frictional force is a linear functional of the history of the velocity $\dot{q}(t)$, and the stochastic force $\xi(t)$ obeys stationary Gaussian statistics. It is fully characterized by the ensemble averages:

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t) \xi(0) \rangle_{cl} \equiv \chi_{cl}(t) \quad (2.15)$$

Where the first equation is giving the time average of the stochastic force and the second is its time correlation average. This second equation is quantifying a time memory.

A classical heat reservoir at temperature T with zero memory time constitutes a white noise source. Then the frictional force is local in time:

$$F_{fric}(t) = -M\gamma\dot{q}(t) \quad (2.16)$$

The stochastic force is correlated according to:

$$\chi_{cl}(t) = 2M\gamma k_B T \delta(t) \quad (2.17)$$

Where k_B is Boltzmann constant and $\delta(t)$ is a delta function.

The dynamics of the damped particle is described by the Langevin equation

$$M\ddot{q} + M\gamma\dot{q}(t) + V'(q) = \xi(t) \quad (2.18)$$

The time local friction proportional to the velocity is usually called Ohmic because of the correspondence with a series resistor in an electrical circuit.

In many cases of practical interest, the heat reservoir exhibits retardation. Then it is a source of colored noise, which has finite memory time, and friction depends on the velocity in the past. The corresponding dynamical equation is the generalized Langevin equation:

$$M\ddot{q} + M \int_{-\infty}^t dt' \gamma(t-t')\dot{q}(t') + V'(q) = \xi(t) \quad (2.19)$$

Since the random force $\xi(t)$ has zero mean, the effect of the reservoir on average is in the memory-friction kernel $\gamma(t)$, which obeys causality, $\gamma(t) = 0$ for $t < 0$. [17]

II. Phenomenological quantum friction models

Once the Hamiltonian is defined it is possible to use the canonical transformation to establish the operator H and then try to resolve the Schrodinger equation. If we consider a system with a particle whose mass is m , moving in a one-dimensional space x with a potential $V(x)$ and a linear frictional force. Ignoring the stochastic process of dissipation, the classical equation of motion for the particle reads as given before as:

$$\frac{dp}{dt} + \gamma p + \frac{\partial V}{\partial x}(x) = 0 \quad (2.20)$$

From this classical equation of motion, the time derivative of the energy $E = p^2/2m + V(x)$ reads:

$$\frac{dE}{dt} = -\frac{\gamma_0}{m} p^2 \quad (2.21)$$

This equation is characterizing the energy dissipation during the dynamical evolution.

In constructing the phenomenological quantum friction models, equations (2.20) and (2.21) should be used as a guiding principle, that is, it is demanded that the time dependence of the expectation values obeys these same equations. Different models are devised to introduce the friction effect in the Schrodinger equation, we are going to review two of these models: the Caldirola-Kanai and the Kostin-Albrecht models.

II.1. The Caldirola-Kanai model

As we mentioned equation (2.20) gives no hint on how it can be translated to a quantum mechanical form. We must then look into more phenomenologically motivated ways to obtain

equation (2.20) and in particular, on those that include some type of effective Hamiltonians. Starting from the Hamiltonian established in equation (2.8) we can use the canonical transformation to achieve the quantal formulation. To pass to the quantum mechanical form of the dissipative problem we can proceed as in going from equation (1.13) to equation (1.15) but now replacing in equation (2.12) P by $-\frac{i\partial}{\partial\bar{x}}$, X by \bar{X} and H by $\frac{i\partial}{\partial t}$ to get the equivalent of the Schrodinger equation but in the dissipative case:

$$i\frac{\partial\bar{\psi}}{\partial t} = e^{-\gamma t} \left(-\frac{1}{2}\frac{\partial^2\bar{\psi}}{\partial\bar{x}^2} \right) + e^{\gamma t}V(\bar{x})\bar{\psi} \quad (2.22)$$

Here $\bar{\psi}$ is not the physical wave function since it is relate to P and X .

In the Caldirola-Kanai model, the Hamiltonian depends explicitly on time t and P is a canonical momentum conjugate to x . The canonical quantization $[x, P] = i\hbar$ with $p = Pe^{-\gamma_0 t}$ leads to the desired equations:

$$\frac{d}{dt}\langle p \rangle + \gamma_0\langle p \rangle + \left\langle \frac{\partial V}{\partial x}(x) \right\rangle = 0 \quad (2.23)$$

$$\frac{d}{dt}\langle E \rangle = -\frac{\gamma_0}{m} \quad (2.24)$$

Here, the expectation value of an operator \mathcal{O} is denoted as $\langle \mathcal{O} \rangle = \int dq \psi^* \mathcal{O} \psi$ with a wave function $\psi = \psi(q, t)$.

Since the Hamiltonian equation (2.9) is Hermitian, the probability is conserved with the continuity equation of:

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial q} e^{-\gamma_0 t} = 0 \quad (2.25)$$

where $\rho = |\psi|^2$ and $J = \left(\frac{\hbar}{m}\right)\Im(\psi^* \frac{\partial \psi}{\partial q})$ are the probability density and the current, respectively, \Im denoting the imaginary part.

Since the kinetic momentum operator in this model depends explicitly on time, the commutation relation between the coordinate and the physical momentum is of the form:

$$[x, p(t)] = i\hbar e^{-\gamma_0 t} \quad (2.26)$$

Hence, the quantum fluctuation disappears as $t \gg 1/\gamma_0$. Consequently, we loss the quantal nature of the problem. One may consider that this unphysical feature can be neglected if one considers only a short time behavior. However, the friction is not active in that time regime,

since the factor $e^{-\gamma_0 t}$ determines how much the momentum is damped, and thus the dynamics may be rather trivial there. This feature of this Hamiltonian expression is rather remarkable as it induces several consequences at physical description of the system. [16]

II.2. The Kostin and the Albrecht models

In the Kostin and the Albrecht models, the momentum operator is kept time-independent, but a non-linear potential W is introduced in the Hamiltonian:

$$H = \frac{p^2}{2m} + V(q) + \gamma_0 W \quad (2.27)$$

$$W_{KO} = \frac{\hbar}{2i} \left(\ln \frac{\psi}{\psi^*} - \langle \frac{\psi}{\psi^*} \rangle \right) = \hbar [\Im \ln \psi - \langle \Im \ln \psi \rangle] \quad (2.28)$$

We can notice that this potential is nothing else than the phase of the wave function.

While in the Albrecht model it is taken as:

$$W_{Al} = \langle p \rangle (x - \langle x \rangle) \quad (2.29)$$

With the canonical quantization, one can derive the equation (2.24) together with

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial q} = 0 \quad (2.30)$$

for both Hamiltonians.

The energy dissipation for the Kostin model is given by:

$$\frac{d}{dt} \langle E \rangle = -\frac{\gamma_0}{m} \langle \left(\frac{mJ}{\rho} \right)^2 \rangle \quad (2.31)$$

Kan and Griffin rederived the Kostin Hamiltonian from a fluid dynamics point of view. In that context, mJ/ρ in equation (2.31) is the kinetic momentum, and hence equation (2.31) is similar to equation (2.21). For the Albrecht model, on the other hand, one obtains

$$\frac{d}{dt} \langle E \rangle = -\frac{\gamma_0}{m} \langle p \rangle^2 \quad (2.32)$$

as is desired. Notice that the energy dissipation is proportional to $\langle p \rangle^2$ in the Caldirola-Kanai and the Kostin models, while it is $\langle p^2 \rangle$ in the Albrecht model. In the classical limit, these quantities are the same to each other, but they may differ in quantum mechanics. [16]

III. Microscopic Approach

The typical approach to describe dissipation is to split the total system in two parts: the quantum system where dissipation occurs, and a so called environment or bath where the energy of the former will flow to wards. The way both systems are coupled depends on the details of the microscopic model, and hence, the description of the bath. To include an irreversible flow of energy (i.e., to avoid Poincarerecurrences in which the energy eventually flows back to the system), requires that the bath contains an infinite number of degrees of freedom. Notice that by virtue of the principle of universality, it is expected that the particular description of the bath will not affect the essential features of the dissipative process, as far as the model contains the minimal ingredients to provide the effect.

III.1. Caldeira–Leggett model

Caldeira–Leggett model is a generic microscopic model describing quantum dissipation. It is a simple semi-empirical model to treat a quantum mechanical anharmonic oscillator which is linearly coupled to a heat bath consisting of a set of non-interacting or independent harmonic oscillators. Hence in this description the bath is a sum of an infinite number of harmonic oscillators, that in quantum mechanics represents a set of free bosonic particles.

The model enables us to investigate dissipation phenomena in the framework of quantum mechanics. Although the model is relatively simple, it enables us to reproduce several properties of realistic dissipative systems without running into difficulties that can appear in the usual way of quantization. Further more, the interaction-independent construction of the model opens up the possibility of application to a wide range of physical systems exhibiting dissipative phenomena. The principle of the model is to consider a system coupled to the environment called bath and which freedom degree causes the energy dissipation. The total Hamiltonian reads then as:

$$H_{tot} = H_s + H_b + V_{coup} \quad (2.33)$$

Where H_s is the system Hamiltonian, H_b is the bath Hamiltonian and V_{coup} is the coupling between the system and the bath. We illustrate the situation in (figure II.1).

The heat bath can be considered as the environment of the physical system, which in Caldeira–Leggett model corresponds to the anharmonic oscillator. As is known the environment plays a crucial role in the appearance of the decoherence phenomenon, the manner by which a quantum system turns effectively into a classical one. Its coupling to the environment makes the physical

system an open quantum system in which quantum dissipation and entanglement may occur, so that the Caldeira-Leggett model may provide a good framework to discuss such phenomena.

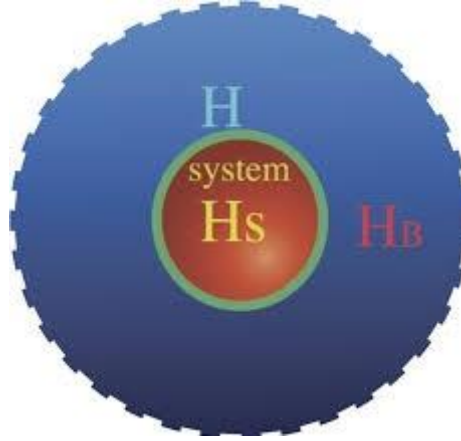


Fig.II.1. A quantum system interacting with the infinitely many degrees of freedom of an environment.

The Hamiltonian reads then:

$$H = \overbrace{\frac{1}{2}M\dot{q}^2 + V(q)} + \overbrace{\sum_{j=1}^N \left(\frac{1}{2}m_j\dot{x}_j^2 - \frac{1}{2}m_j\omega_j^2 x_j^2 \right)} + \overbrace{q \sum_{j=1}^N g_j x_j} - q^2 \sum_{j=1}^N \frac{g_j^2}{2m_j\omega_j^2} \quad (2.34)$$

Where g_j are constants.

The first bloc corresponds to the Hamiltonian of a quantum particle of mass M and momentum \dot{q} , in a potential $V(q)$ at position q . The second bloc describes the bath as an infinite sum of harmonic oscillators with masses m_j and momentum \dot{x}_j , at positions x_j . ω_j are the frequencies of the harmonic oscillators. The next bloc describes the way the system and the bath are coupled. The last term is simply a counter term not depending on the oscillator coordinates. The physical reason for the introduction of such term is to let the minimum of the Hamiltonian, and thus of the energy, correspond to the minimum of the external potential $V(q)$. This term must be included to ensure that dissipation is homogeneous in all space. As the bath couples to the position, if this term is not included the model is not translationally invariant, in the sense that the coupling is different wherever the quantum particle is located. This gives rise to an unphysical renormalization of the potential, which can be shown to be suppressed by employing real potentials.

Going in all the details of the resolution of this model is beyond the framework of this study. It is however interesting to report that a propagator can be derived from the Hamiltonian and a solution can be deduced for this model. The remarkable point to notice is that the only feature of the bath that enters this propagator is its spectral density.[14]

IV. Motion of wave packet with dissipation

In this section we are going to exploit the already given formalism to illustrate how the motion of a Gaussian wave packet is modified when the medium is characterized by a constant rate of friction. We will expose the solution of the time dependent Schrodinger equation only for the case of the Caldirola-Kanai model of the friction. As the Hamiltonian was established for the variable X and P , we will note the wave function as $\bar{\psi}(X, t)$ as it is related with the physical $\psi(x, t)$ by a non-unitary connection. We now restrict ourselves to the case when $V(X) = 0$ and consider again the problem of the previous section in the presence of dissipation. This implies finding the $\bar{\psi}(X, t)$ solution of

$$i \frac{\partial \bar{\psi}}{\partial t} = e^{-\gamma t} \left(-\frac{1}{2} \frac{\partial^2 \bar{\psi}}{\partial X^2} \right) \quad (2.35)$$

$$\bar{\psi}(X, t = 0) = f(X) \quad (2.36)$$

Where $f(x)$ is the initial Gaussian wave packet as given in the previous chapter but this time as function of X .

If we multiply equation (2.35) by $e^{\gamma t}$ we can replace on the left hand side the time variable t by: $\tau = \frac{1}{\gamma}(1 - e^{-\gamma t})$ and as it has the property that for $t = 0, \tau = 0$, our problem reduces to finding the solution of:

$$i \frac{\partial \bar{\psi}}{\partial \tau} = -\frac{1}{2} \frac{\partial^2 \bar{\psi}}{\partial X^2} \quad (2.37)$$

$$\bar{\psi}(X, \tau = 0) = f(X) \quad (2.38)$$

Which is exactly the same problem that we have discussed in the previous chapter but in which we have to substitute t by τ and x by X .

Thus, the absolute value squared of the solution of equation (2.37) is:

$$|\bar{\psi}(X, \tau)|^2 = \frac{1}{\sqrt{\pi}a\sqrt{1+\frac{\tau^2}{a^4}}} e^{-\frac{(X-x_0-p_0\tau)^2}{a^2\left(1+\frac{\tau^2}{a^4}\right)}} \quad (2.39)$$

We could discuss the dependence of $|\bar{\psi}(X, \tau)|^2$ on X, τ exactly in the same way as we did in the previous chapter for the non-dissipative problem, but in order to do comparison we have to express this probability density in terms of the physical variables x, p rather than X, P and also consider the non-unitary change from $\bar{\psi}$ to ψ and renormalize the latter.

For the coordinate and momentum observables we have:

$$X = x \text{ and } P = pe^{\gamma t} \quad (2.40)$$

which stresses the non-canonical relation between x, p and X, P .

Making use of the Hamiltonian-Jacobi equation in these variables and Schrödinger relation between the action S and the wave function ψ one obtains:

$$\bar{\psi} = \psi e^{\gamma t} \quad (2.41)$$

which is clearly a non-unitary kind of transformation. From equation (2.41) we have that:

$$|\psi(x, t)|^2 = |\bar{\psi}(X, \tau)|^2 e^{-\gamma t} \quad (2.42)$$

and replacing the first term in the right hand side by its value in equation (2.35) we obtain for the problem with dissipation that:

$$|\psi(x, t)|^2 = \left[\frac{1}{\sqrt{\pi}\sigma\sqrt{\left(1+\frac{\tau^2}{\sigma^4}\right)}} \right]^{-e^{\gamma t}} \exp \left[-\frac{(x-x_0-p_0\tau)^2}{e^{\gamma t}\sigma^2\left(1+\frac{\tau^2}{\sigma^4}\right)} \right] \quad (2.43)$$

This is not yet the probability density of finding the particle at point x at time t as the normalization of the wave function was affected by the non-unitary transformation of equation (2.41). In our present problem, where $|\psi(x, t)|^2$ is a gaussian of width $\sqrt{e^{\gamma t}\sigma^2(1+\tau^2\sigma^{-4})}$, we just have to replace the first bracket in equation (2.43) by the inverse of this width and keeping the factor $\left(\frac{1}{\sqrt{\pi}}\right)$ we get:

$$P(x, t) \equiv \frac{1}{\sqrt{\pi}e^{\frac{\gamma t}{2}}a\sqrt{\left(1+\tau^2a^{-4}\right)}} \exp \left[-\frac{(x-x_0-p_0\tau)^2}{e^{\gamma t}a^2\left(1+\frac{\tau^2}{a^4}\right)} \right] \quad (2.44)$$

The $P(x, t)$ is now the normalized probability density for the problem with dissipation for finding the particle at the point x and time t .

A comparison between the evolution in time of the wave packet for the case of conservative and non conservative system is presented in (figure II.2). As expected, the dissipative case is retarded compared to the case with no dissipation and the spreading of the Gaussian is also

more important for the dissipative case. The maximum of the Gaussian is also smaller for the dissipative system. These results can be induced from a straight forward comparison between the two mathematical formulas. [12]

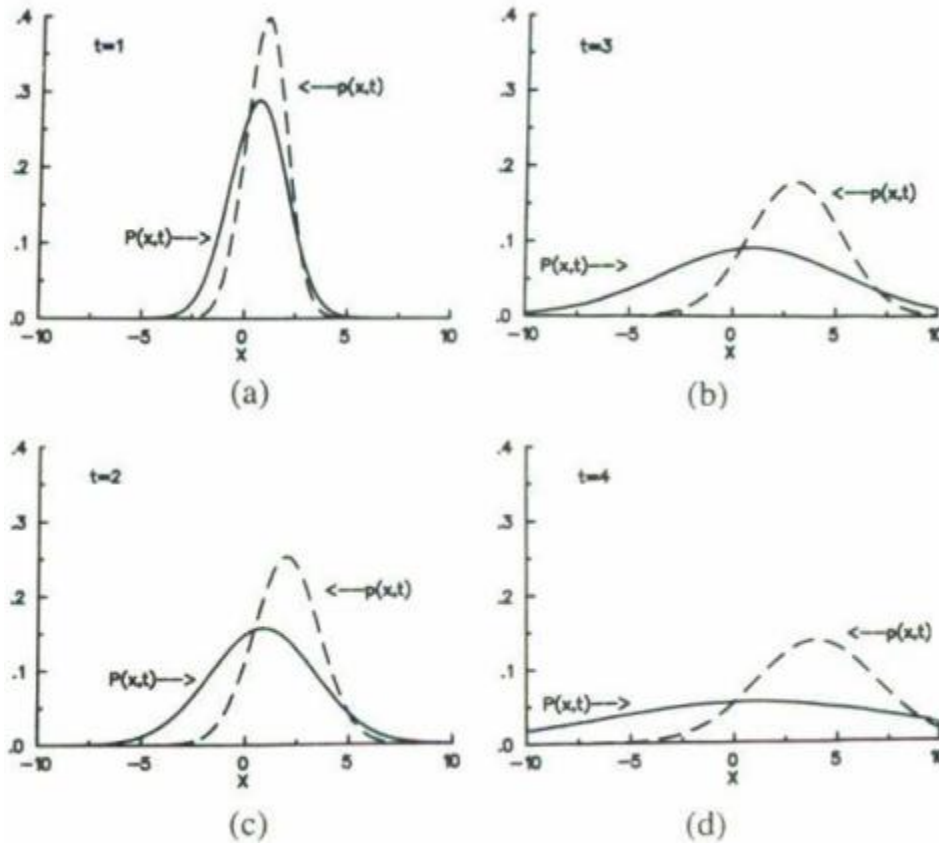


Fig.II.2. Comparison for four different sample of time between the dissipative case (full line) and the non dissipative case (dashed line) for the motion of a Gaussian wave packet

CHAPTER III: IMPLEMENTATION AND EVALUATION

I. Introduction

We have presented in the previous chapters through some theoretical developments, two main practical results related to the propagation of a Gaussian wave packet:

-An analytical expression for the motion of the wave packet with no dissipation taken into consideration.

-An analytical expression for the motion of the wave packet in the case of the propagation in a medium with a constant friction factor.

We have to bear in mind that these results are established in the case of free motion i.e., no potential of any kind is assumed. However, the case of a motion in particular potentials are the most interesting cases that we encounter in reality. In these cases, however it is impossible to reach an analytical solution and the only alternative is to resolve the problem numerically. The physical situation in which we are interested is the case of particles that could be electrons or nuclei penetrating a barrier or a general collision problem. The particles are represented by a Gaussian wave packet and to start, we are considering the penetration of a simple square barrier. For the case of dissipative systems, the friction should be limited to the barrier region and for this, the Caldirola-Kanai model is adopted for the friction study. We use FORTRAN software for the coding and some numerical recipes are needed to overcome the non linearity encountered in this kind of problems. To test the efficiency of our program, we compare the numerical results with the analytical expressions in the case with no dissipation and the case of a medium with a constant friction. The validity of these tests will assure mainly the validity of the results in the case of the barrier penetration.

II. Numerical strategy

To resolve the time dependent Schrödinger equation several methods are proposed in the literature. The most popular approach is maybe the Crank-Nicolson scheme where the propagator of the solution at time zero to ulterior times is written in a symmetric form assuring the unconditional stability of this method. However, this strategy is only possible in the linear form of the Schrödinger equation. Assuming the Caldirola-Kanai model for the dissipative regime we can straight forwardly notice that the Schrödinger equation is no longer linear and more investment should be devoted to the elaboration of the solution encompassing not only the theoretical formulation but also management of the computer resources.

Let us explicit more the situation. The origin of the non linearity comes from the fact that the propagator $U(t, t_0)$ of the solution in the Schrödinger equation without friction is given by:

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle \quad (3.1)$$

Where:

$$U(t, t_0) = e^{\frac{-i}{\hbar}H(t-t_0)}$$

H is the Hamiltonian of the system. Hence it is obvious that to reach the solution $|\Psi(t)\rangle$ at any instant t it is sufficient to evaluate the propagator $U(t, t_0)$. In the Cayley or the Crank Nicolson method a symmetric form of the exponential is developed to the first order and results in:

$$\psi^{t_{j+1}} = \frac{I-iH}{I+iH} \psi^{t_j} \quad (3.2)$$

The discretization of this formula will lead us to the evaluation of a tridiagonal matrices which are the same at each time iteration.

However, when we use the Caldirola-Kanai approach the Hamiltonian becomes time-dependent and this non linearity will violate the superposition principle. In addition, in the original models for quantum friction, the friction constant γ_0 is treated to be a constant. When considering friction in a collision problem, however, we have to introduce a friction form factor $f(x)$, since the energy dissipation occurs only during interaction. That is, the form factor $f(x)$ vanishes outside the range of the potential $V(x)$. A naive replacement of γ_0 in the model Hamiltonians with $\gamma_0 f(x)$ does not work due to the x dependence in the form factor. Alternatively, in this study we consider a time dependent friction coefficient $\gamma(t)$ which vanishes after the interaction. In the simple form of $\gamma(t) = \gamma_0 f(\langle q \rangle_t)$ the dissipation continuously occurs even after the interaction if an incident wave is equally bifurcated into transmitted and reflected waves. To avoid this undesired behavior, we choose the form:

$$\gamma(t) = \gamma_0 \langle f(q) \rangle_t \quad (3.3)$$

For the Caldirola-Kanai model, on the other hand, the following modification is necessary:[16]

$$H = \frac{\pi^2}{2m} e^{-\int_0^t dt' \gamma(t')} + e^{\int_0^t dt' \gamma(t')} \quad (3.4)$$

Here we have assumed that the initial time is $t = 0$. The uncertainty relation is now changed from equation (2.26) to:

$$[q, p(t)] = i\hbar e^{-\int_0^t dt' \gamma(t')} \quad (3.5)$$

Instead of using the Crank-Nicolson scheme, we carry out the numerical integration in the following way. The discretized Schrödinger equation may be given at the n^{th} time grid by:

$$i\hbar \frac{\psi^{n+1} - \psi^n}{\Delta t} = \frac{H^{n+1}\psi^{n+1} + H^n\psi^n}{2} \quad (3.6)$$

Here H is the Hamiltonian which depends on ψ . In our calculation, we simply neglect the time dependence of the Hamiltonian and obtain:

$$i\hbar \frac{\psi^{n+1} - \psi^n}{\Delta t} = H^n \frac{\psi^{n+1} + \psi^n}{2} \quad (3.7)$$

Then the discretization of the second derivative of the kinetic operator in the Hamiltonian gives:

$$\left(\frac{d^2\psi}{dx^2}\right)_{x_n} = \frac{\psi_{x_{n+1}} - 2\psi_{x_n} + \psi_{x_{n-1}}}{a^2} \quad (3.8)$$

And the whole equation can be put in following form:

$$\psi^{n+1} = D_1^{-1} D_2 \psi^n \quad (3.9)$$

Where:

$$D_1 = \begin{pmatrix} \gamma_1 & \alpha & & & & & \\ \alpha & \gamma_2 & \alpha & & & & \\ & \alpha & \gamma_3 & \alpha & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \alpha & \gamma_{N-1} & \alpha & \\ & & & & \alpha & \gamma_N & \end{pmatrix}$$

And:

$$D_2 = \begin{pmatrix} \xi_1 & -\alpha & & & & & \\ -\alpha & \xi_2 & -\alpha & & & & \\ & -\alpha & \xi_3 & -\alpha & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\alpha & \xi_{N-1} & -\alpha & \\ & & & & -\alpha & \xi_N & \end{pmatrix}$$

With: $\alpha = \frac{i\Delta t}{4\Delta x^2}$, $\gamma_j = 1 - \beta_j$, $\xi_j = 1 + \beta_j$

And $\beta_j = \frac{i\Delta t}{2} \left(\frac{1}{\Delta x^2} e^{-\gamma(t)*t} + V_j e^{\gamma(t)*t} \right)$

We consider here: $\hbar = m = 1$

This final form is used in our program to follow the evolution of the Gaussian wave packet.

III. Coding strategy and implementation

To translate the numerical results established at the end of the previous section we are using FORTRAN software for the coding and the LAPACK libraries for the routines of diagonalization, matrix-matrix product and matrix-vector product. Besides being very commonly used by the physicists community, the FORTRAN software is a very versatile language allowing through its object orientation and low structure plenty of manipulations that are not possible with other languages. When FORTRAN coding is coupled with LAPACK libraries which are ready to use FORTRAN routines, coding becomes easier and more compact.

The program includes an input part where we assign values to some parameters whether physical or needed for the structure of the program as for example the friction constant, parameters for the initial wave packet, assignment of matrices elements of the Hamiltonian... and the spatial and temporal paces (Δx and Δt)... For each iteration we have the evaluation of inverse matrix D_1^{-1} then the matrices product $D_1^{-1}D_2$ and then the matrix-vector product $D_1^{-1}D_2\psi^n$. Where for this operation we are using the complex-valuated routines: cgetrf, cgetri, cgemm and cgemmv. These different operations could be summarized by the flowchart of (figureIII.1)

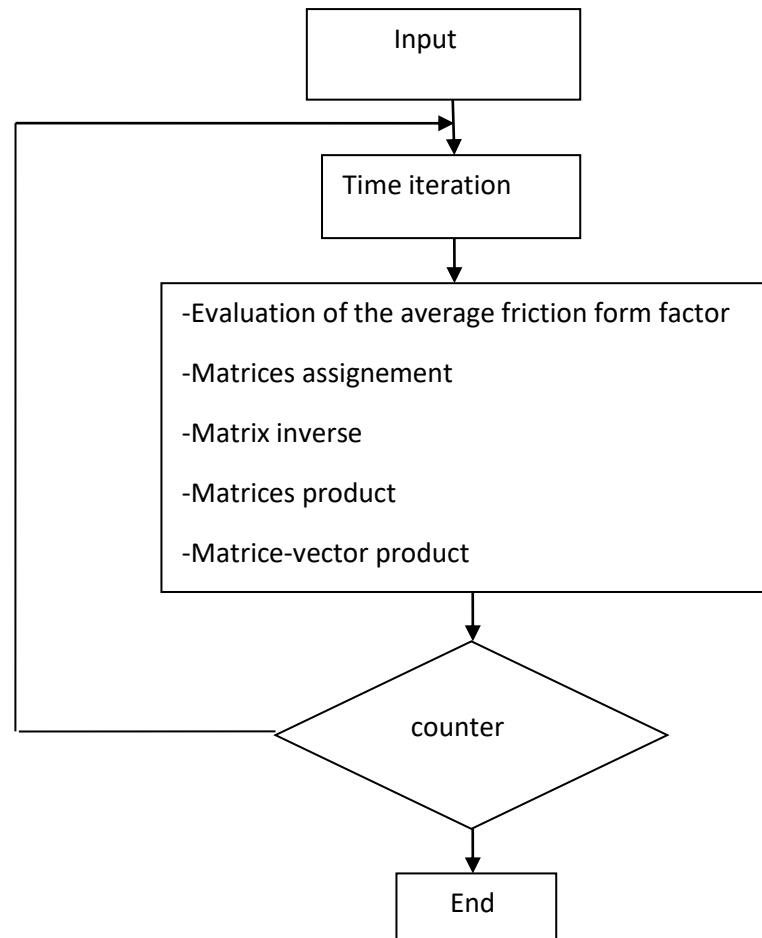


Fig.III.1. flowchart of the elaborated program

The program is outputting formatted files for gnuplot. It is possible then to create an animation that allows the observation of the evolution of the wave packet across time. Only snapshots of this animation are captured to sketch the main features of the process. An example of these snapshots is illustrated on (figure III.2) and (figure III.3). On (figure III.2) we can see the natural spreading of the Gaussian wave packet as it evolves in time when no potential is considered. The (figure III.3) on the other side gives an example of the impact of the wave packet on a square potential and we can see clearly the bifurcation of the wave in a reflected part at the left and a transmitted part on the right and a resonant part at the barrier. This is clearly depicting a tunnel passage of the barrier.

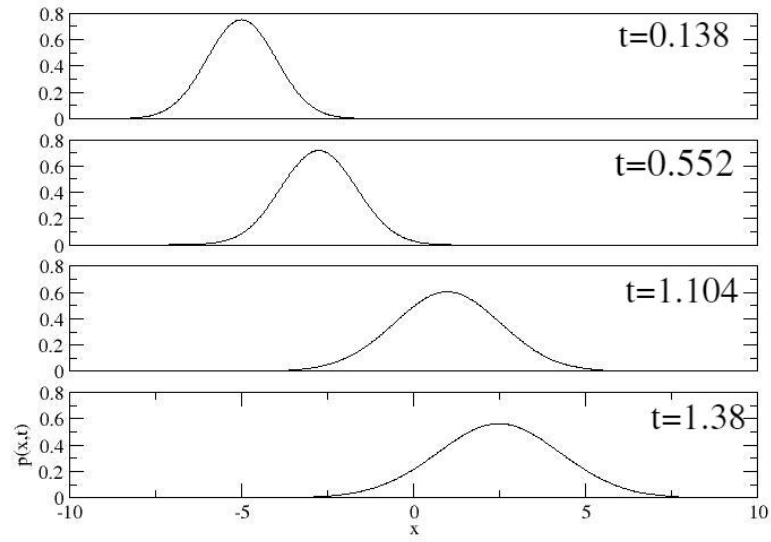


Fig.III.2. Snapshots of the evolution of the free Gaussian wave packet without dissipations

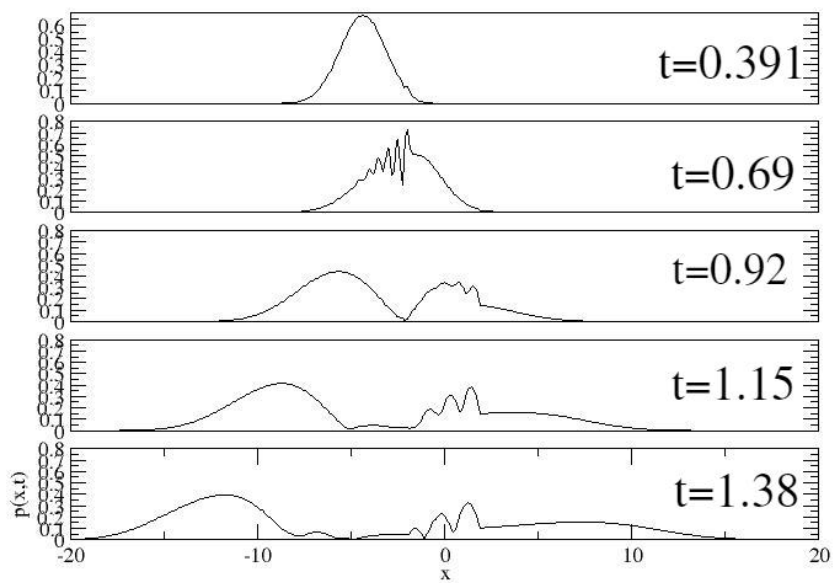


Fig.III.3. Snapshots of the evolution of the Gaussian wave packet without dissipations through a square barrier.

IV. Tests and the program validation

It is important to test our program for case where analytical results exist. This benchmark of tests will allow us to be confident about the results established for the other cases where no analytical results exist. For this we are going to use the two analytical results presented before for the case with no friction and the case of a medium with a constant friction factor.

IV.1. Analytical-numerical comparison for the case without friction

As we have showed in the first chapter an analytical solution for the propagation of a Gaussian wave packet without dissipation exists and the probability density is as:

$$p(x, t) \equiv |\psi(x, t)|^2 = \frac{1}{\sqrt{\pi}\sigma\sqrt{1+\frac{t^2}{\sigma^4}}} \exp\left\{-\frac{(x-x_0-p_0t)^2}{\sigma^2\left(1+\frac{t^2}{\sigma^4}\right)}\right\} \quad (3.10)$$

To perform the comparison of this result with our program we are setting $\sigma = 1$, $p_0 = 10$ and $\gamma = 0.00$, $\Delta x = 0.05$ and $\Delta t = 0.00023$ (all in atomic units)

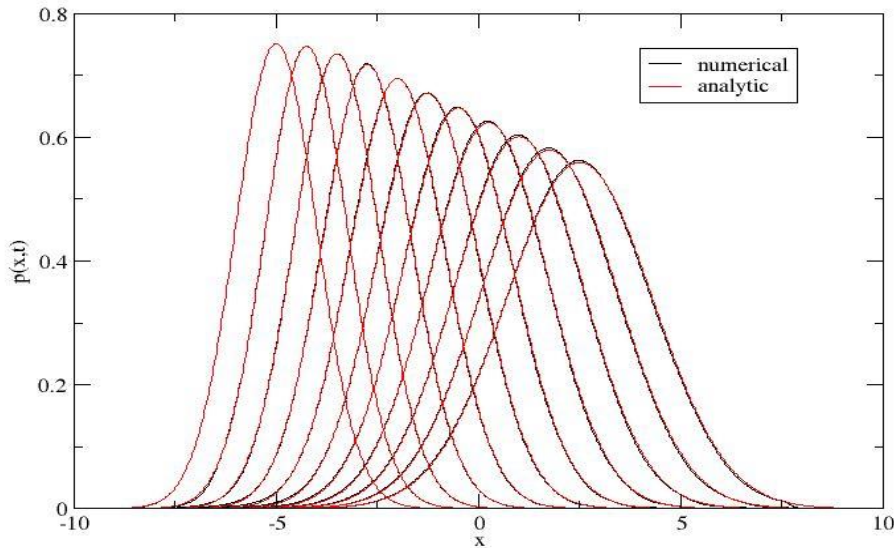


Fig.III.4. Numerical-analytical comparison for a Gaussian wave packet with no dissipation

The comparison of the wave packet for equidistant time intervals equal to $600 * \Delta t$ is illustrated in (figure III.4). We can see clearly that our numerical results agree perfectly well with the

analytical results. Let us however report that it is important to take Δx as small as the value given previously to assure the stability of our calculation and to avoid cumulating numerical error originating from the assumption that the Hamiltonian is time independent between two time iterations. We could establish this result quite easily using the Crank-Nicolson method with no numerical constraint but we are rather interested in the limit of our non linear program in the case of systems with no dissipations.

IV.2. Analytic-numerical with friction $\gamma = 1$

Similarly, we have given the analytical expression of the density probability of the Gaussian wave packet in case where the whole medium is characterized with a constant friction factor as:

$$P(x, t) \equiv \frac{1}{\sqrt{\pi} e^{\frac{\gamma t}{2}} \sigma \sqrt{(1 + \tau^2 \sigma^{-4})}} \exp \left[-\frac{(x - x_0 - p_0 \tau)^2}{e^{\gamma t} \sigma^2 \left(1 + \frac{\tau^2}{\sigma^4}\right)} \right] \quad (3.11)$$

To perform the calculation, we are setting: setting $\sigma = 1$, $p_0 = 10$ and $\gamma = 1.00$, $\Delta x = 0.05$ and $\Delta t = 0.00023$ (all in atomic units).

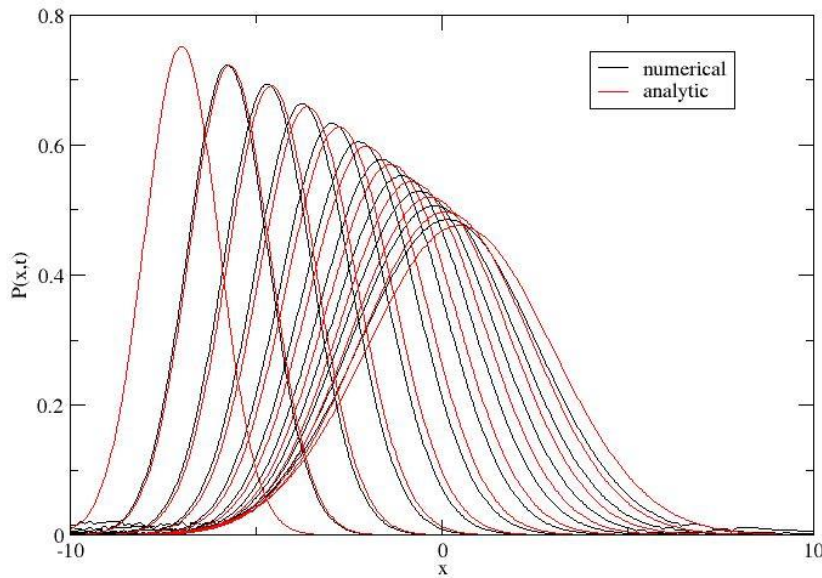


Fig.III.5. Numerical-analytical comparison for a Gaussian wave packet with a friction factor $\gamma = 1.00$

The wave packet for equidistant time interval of $600 * \Delta t$ is illustrated in (figure III.5). In these calculations we are setting $\gamma = 1.00$ without averaging this value between two time iterations.

We can notice the perfect agreement for the first curves and a small disagreement starts to appear for the last curves as a result of the accumulation of a numerical error. We have checked that the shift is related to the value of Δx by seeing that the shift is smaller for a smaller Δx . It was unfortunately impossible to go below the value mentioned above because of the limitation of computer memory resources. We can however ascertain that besides this numerical shortcoming our program reproduces quite well the analytical results. We can then move to the following step of this study where we perform the calculation for a square barrier potential.

V. Penetration of square barrier potential

For this section we are considering a square barrier potential given by the following formulation:

$$V(x) = \begin{cases} \frac{p_0^2}{2} & -x_b < x < x_b \\ 0 & \text{otherwise} \end{cases}$$

Where: $x_b = 2ua$ and p_0 is the initial momentum of the wave packet

The shape of this potential is illustrated in (figure III.6)

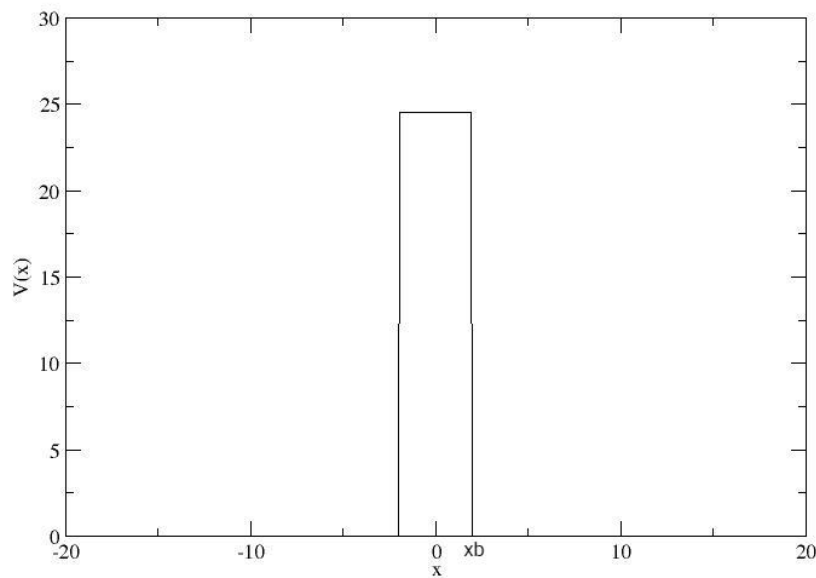


Fig. III.6. Square barrier as used in this study

V.1.Dissipation effect on the barrier transmission:

In this first calculation we are going to show in a qualitative way the effect of the friction on the portion of the wave packet that is transmitted through the barrier. The friction is limited only to the region of the barrier through the averaging process that we have explained before. We are taking the case with $\gamma=0$ as the reference for our calculation and then we introduce friction gradually through increasing the value of γ and keep track of what is happening to the wave packet. Through the snapshots of (figure III.6) that starting from the same wave packet we end up with different bifurcation schemes and this is due mainly to the effect of the friction at the barrier. It is clear from this illustration that the dissipation leads to the decrease of the proportion of the transmitted wave packet.

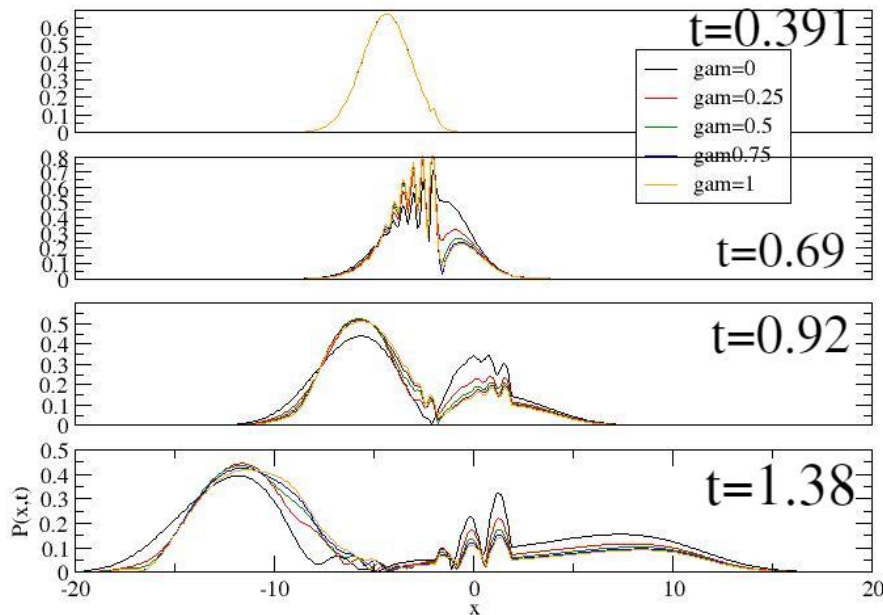


Fig. III. 7. Snapshots of the evolution of the wave packet with different friction factors.

In a more quantitative manner we can see on (figure III.8) the transmission percentage versus time for different friction constants that the transmission decreases clearly with increasing friction.

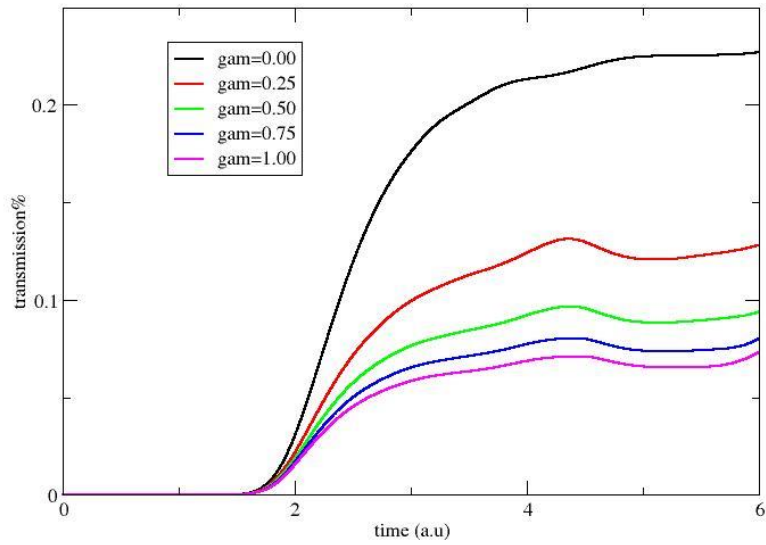


Fig. III.8. Transmission percentage versus time for different friction constants

In summary we can state that our appropriate handling of a realistic case of dissipative systems which is the penetration of a square barrier can lead to conclusive results. The consideration of friction was performed through Caldirola-Kanai model. However, the implementation of this model at the numerical level for study case requires a special treatment of the friction rate as it is only limited to the barrier region. The final results illustrate as expected a direct correlation between the friction rate and the barrier transmission.

Conclusion

The main aim of this study is to analyze the effect of the friction on the wave packet transmission through a square barrier potential. To reach this goal, we started by presenting a theoretical review of the physics for non conservative and conservative systems. It was obvious through that very short review that the incorporation of dissipation in the dynamical evolution of the physical system is quite ubiquitous.

It was important in a second place to illustrate the physical advantages behind the use of the wave packet for describing the system and in which extent this more appropriate physically.

The main contribution of this study is the build of a FORTRAN program that implements the numerical aspects of our problem. Particularly the non linearity of the equation was clearly addressed and implemented.

In order to quantify the correctness of our numerical tool, a systematic comparison with well established analytical cases was performed. The comparison is satisfactory within the numerical constraints imposed by the computer resources.

For the realistic case of the square barrier transmission, we used our program in order to evaluate the effect of the friction on the transmission rate. It was clear from the qualitative and quantitative results that the transmission is decreasing with increasing damping rate.

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Abstract:

Friction is an important player in any dynamical evolution of the physical system. The introduction of friction in the formalism for classical system is quite complicated and relies essentially on phenomenological approaches. Situation becomes even more difficult for quantum systems where the correspondence relation for the Hamiltonian is not obvious. In this master project we are attempting to review the theoretical basis for the introduction of friction in classical and quantum system. We are specially interested in the effect of friction on the transmission of a wave packet tunneling through a square barrier.

Résumé:

Les frottements jouent un rôle important dans l'évolution dynamique de tout système physique. L'introduction des frottements pour les systèmes classiques est assez compliquée et repose essentiellement sur les approches phénoménologiques. La situation devient plus difficile pour les systèmes quantiques où les relations de correspondance pour le Hamiltonien n'est pas évidentes. Dans ce projet de master on tente de revoir les bases théoriques pour l'introduction des frottements dans les systèmes classiques et quantiques, on est intéressé spécialement par l'effet des frottements sur la transmission du paquet d'onde qui passe par effet tunnel à travers une barrière carrée.

الملخص:

يلعب الاحتكاك دورا مهما في التطور الديناميكي لأي نظام فيزيائي. ادخال الاحتكاك في التعبير الرياضي للأنظمة الكلاسيكية معقد إلى حد كبير ويعتمد أساسا على مقاربات ظواهرية. يصبح الأمر أكثر تعقيدا من أجل الأنظمة الكمية أين تكون علاقات الربط للهاملتونين أقل وضوحا. في هذا العمل نحاول تقديم الأسس النظرية لادخال الاحتكاك في الأنظمة الكلاسيكية والكمية. يتعلق الأمر خصوصا بدراسة أثر الاحتكاك على اختراق حزمة الأمواج التي تمر بفعل النفق من خلال حاجز مربع.