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Trabajo Fin de Máster:

DINÁMICA NO LINEAL DE SISTEMAS CUÁNTICOS ABIERTOS

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Abstract:

Open quantum systems can be represented as a system plus environment from the Caldeira-Leggett Hamiltonian. The Langevin equation of motion associated with this Hamiltonian is obtained. This equation of motion is transformed into the Schrödinger-Langevin equation by two methods: the Kostin procedure, which is generalised, and the Nottale scale relativity method. The Schrödinger-Langevin equation is applied to the description of quantum Brownian motion in the Bohm interpretation by considering as possible solutions of the equation Gaussian wave packets with and without stretching factor. From this motion, the quantum stochastic trajectories, the mean square displacement, the diffusion coefficient and the associated uncertainty product are obtained.

Resumen:

Los sistemas cuánticos abiertos se pueden representar como un sistema más entorno a partir del Hamiltoniano de Caldeira-Leggett. De este Hamiltoniano, se obtiene la ecuación de Langevin del movimiento asociada. Esta ecuación del movimiento se transforma en la ecuación de Schrödinger-Langevin mediante dos métodos, el procedimiento de Kostin, el cual se generaliza, y el método de relatividad de escala de Nottale. La ecuación de Schrödinger-Langevin se aplica a la descripción del movimiento cuántico Browniano en la interpretación de Bohm considerando como posibles soluciones de la ecuación paquetes de onda Gaussianos con y sin factor de stretching. De este movimiento se obtienen las trayectorias estocásticas cuánticas, el desplazamiento cuadrático medio, el coeficiento de difusión y el producto de incertidumbre asociado.

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1 Introduction

Real systems are influenced by the outside world and the closed description of quantum mechanics does not cover all situations. These situations are studied by open quantum systems, which are local quantum systems interacting with an external quantum system called bath or environment. The local system and the bath have unitary evolution and the bath coordinates are deleted to obtain a closed equation for the total dissipative system. The friction between the two parts of the system displays a transfer of energy from the quantum system to the bath. The dynamic of open quantum systems is stochastic, it means the evolution of the system has a random evolution, and it comes from the environment is uncontrolled. There are three main approaches to the open quantum systems: (i) effective time dependent Hamiltonian, (ii) non-linear Schrödinger equation and (iii) the system plus bath model.

The purpose of this work is the theoretical development from the starting Hamiltonian of the system plus bath to the non linear Schrödinger equation associated with open quantum systems. This non linear equation is determined by three ways: the Kostin procedure, its generalization and the scale relativity method.

The system plus bath model for a one dimensional system considered to start the theoretical development of this work is the Caldeira-Leggett Hamiltonian [1]. The system evolution for this Hamiltonian can lead to the generalized Langevin equation.

The Langevin equation is a stochastic differential equation describing a time evolution of a set of the degrees of freedom. This equation was introduced by Langevin in 1908 to describe the motion of the Brownian particle according to Newton's laws [2].

The Brownian motion was first described by Robert Brown in 1827 when he observed under a microscope pollen grains immersed in water and their movement was a rapid oscillatory motion. The main experimental features observed for this motion are the irregularity, the independence of motion between particles, the density of the particles does not matter, the motion never ends and the higher activity of the system with lower particles, lower fluid viscosity or higher temperatures. Einstein predicted for longer times the motion will be a diffusion motion.

The Brownian experimental features serve to build the Langevin equation in function of the Newton laws. Then, there are considered two forces, a dynamical friction force

and a rapidly fluctuating force. The fluctuating force comes from the impacts of the molecules of the liquid on the particle, described as a white noise. The white noise is an approximation for a process with correlation time approaching to 0.

The generalized Langevin equation is related to a non linear Schrödinger equation for a open quantum system. In this situation, the non-linear Schrödinger equation is known as Schrödinger-Langevin equation or Kostin equation and the dynamics of open quantum systems can be described by this equation. The development to obtain the non linear equation from the Langevin equation is demonstrated by Kostin [3] with the Heisenberg position and momentum operators. This Kostin procedure is also generalised in this work [4].

Another way to obtain the Schrödinger-Langevin equation is the scale relativity method. This theory is developed by Laurent Nottale [5, 6] in which the Schrödinger equation is obtained from the Newton laws with the principle of scale covariance. This theory considers a differentiable space-time with fractal behaviour, which is not shown in the classical regime. In this space-time, the quantum trajectories are continuous but not differentiable. The quantum regime is divided in two sides associated with the differentiable side and the fractal side. This theory describes Brownian motion with a fractal dimension $D_F = 2$ [7] and considers the stochastic motion of particles associated with the fractal space-time.

After the theoretical development, the purpose is the application of this work to the Brownian-Bohmian motion, a Brownian motion described by the Bohm interpretation of the quantum mechanics. This motion is described for a Gaussian wave packet and for a stretched Gaussian wave packet and the equation of motion for the center of the wave packet and the width are obtained for the free particle. The importance of the stretched Gaussian wave packet is that it has not been studied before in the literature. For this reason, their results are compared to the results for the Gaussian wave packet.

The quantum mechanics interpretation in this work is the Bohm interpretation [8, 9]. This interpretation explains the mechanics of the quantum systems in a closed set of possible trajectories. Moreover, the trajectory is deterministic, but the probability is in which trajectory the particle follows. The points of the configuration space can be followed along the space, unlike the standard quantum mechanics. The difference with the Newton equations is that a quantum mechanical potential associated with

the wave function is considered. This interpretation is associated with the description of quantum theory in hidden variables since in macroscopic physics the position and momentum of each atom is not considered. For example, the uncertainty product is understood like a problem to determine the trajectory followed by the particle along the motion with the initial conditions.

The Bohm interpretation applied to the Schrödinger-Langevin equation gives the Schrödinger- -Langevin-Bohm equation. It is obtained from the wave function described in polar form. For this equation, two types of solution are considered, the Gaussian wave packet and the stretched Gaussian wave packet which give the same types of evolution for their respective wave packet centre and width. The wave packet centre corresponds to the classical Langevin equation while the width evolution is described with the damped Pinney equation, it is a Pinney equation with a friction term. This equation can not be solved analytically while the solution for the undamped Pinney equation was proposed in [10]. The Langevin equation gives random trajectories for the individual particle because there is a stochastic force. For this reason, it is used to describe the motion averaged quantities.

The averaged quantities to describe the motion for the free particle Gaussian and stretched Gaussian wave packet evolution is the diffusion coefficient and the mean squared displacement in the classical and quantum counterparts. The diffusion coefficient is a key concept for the Brownian motion and must fulfill Einstein relation. The diffusion coefficient is the rate at which the solute moves in the solvent. The mean squared displacement is the average of the random trajectories the particle can follow in the motion. The uncertainty product is also represented because it allows the observation of the Heisenberg minimum uncertainty product to be fulfilled over all time.

The organization of this work is in section 2 the theoretical development with the following subsections. The section 2.1 gives a general description of the Caldeira-Legget Hamiltonian. The next section 2.2 develops the Langevin equation of motion associated to the Caldeira-Legget Hamiltonian. The section 2.3 describes the two different methods to obtain the Schrödinger-Langevin equation from the Langevin equation with the generalization of the Kostin procedure. The section 3 consists of the application for the Brownian-Bohmian motion. The Gaussian wave packet is developed in section 3.1

while stretched Gaussian wave packet in section 3.2. In section 3.3 the main feature of the Brownian motion for a free particle is described for the two wave packets. The results of the simulations are in section 4 and the final conclusions of this work are in section 5. An appendix in section 6 is included with the relation of probability current and the explained expected position.

2 Theoretical development

2.1 Caldeira-Leggett Hamiltonian

The system under study is coupled to a huge environment composed by a bath of harmonic excitations around a steady state. The open system is divided into the system, the reservoir and the interaction between the two. In this terms, the Hamiltonian can be separated as

$$H = H_S + H_R + H_I \quad . \tag{1}$$

The description of the different Hamiltonian terms are for the system

$$H_S = \frac{P^2}{2M} + V(q) \quad , \tag{2}$$

for the reservoir compound of a bath with N harmonic oscillators

$$H_R = \sum_{\alpha=1}^{N} \left(\frac{p_\alpha^2}{2m_\alpha} + \frac{1}{2} m_\alpha w_\alpha^2 x_\alpha^2 \right) \tag{3}$$

and for the interaction between the system and the reservoir which is described by the reservoir coordinates

$$H_I = -\sum_{\alpha=1}^{N} F_\alpha(q) x_\alpha + \Delta V(q) \quad . \tag{4}$$

The extra term $\Delta V(q)$ depends on the reservoir variables m_α , w_α and the force $F_\alpha(q)$. The term does not depend on the positions of the reservoir, x_α. The origin of the introduction in the description of the potential term $\Delta V(q)$ is to compensate the renormalization of the potential $V(q)$ caused by the linear coupling at the position x_α for the interaction Hamiltonian.

Disregarding the extra potential term, $\Delta V(q)$, the minimum position x_α in the

potential of the global system for the coordinate q is [1]

$$x_\alpha = \frac{F_\alpha(q)}{m_\alpha w_\alpha^2} \quad . \tag{5}$$

When the extra potential term is considered, it is necessary to consider the renormalization of the potential caused by the coupling, giving the following effective potential with a harmonic approximation of the position

$$V_{ef}(q) = V(q) - \sum_{\alpha=1}^{N} \frac{F_\alpha^2(q)}{2m_\alpha w_\alpha^2} \quad . \tag{6}$$

If a linear force is considered $F_\alpha(q) = c_\alpha q$, the second term of the effective potential generates the following frequency shift [1]

$$(\Delta w)^2 = -\sum_{\alpha} \frac{c_\alpha^2}{M m_\alpha w_\alpha^2} \quad , \tag{7}$$

and generates the following perturbation of the frequency around the minimum of the frequency, w_0^2, as

$$w_{ef}^2 = w_0^2 + (\Delta w)^2 < 0 \quad . \tag{8}$$

This form of the effective potential with a value less than 0 changes the potential in a qualitative way. If a dissipation effect is introduced and it is not only a renormalization of $V(q)$, there must be a balance to the second term of the effective potential as

$$\Delta V(q) = \sum_{\alpha=1}^{N} \frac{F_\alpha^2(q)}{2m_\alpha w_\alpha^2} \quad . \tag{9}$$

After this explanation about the dissipation effect, the three components of the Hamiltonian Eq.(2), Eq.(3) and Eq.(4) in Eq.(1) considering a separable force ($F_\alpha(q) = c_\alpha F(q)$) are

$$H = \frac{P^2}{2M} + V(q) + \frac{1}{2}\sum_{\alpha=1}^{N}\left(\frac{p_\alpha^2}{m_\alpha} + m_\alpha w_\alpha^2\left(x_\alpha - \frac{c_\alpha F(q)}{m_\alpha w_\alpha^2}\right)^2\right) \quad . \tag{10}$$

If the separable force is a linear force ($F_\alpha(q) = c_\alpha q$), the Caldeira-Leggett Hamiltonian

is

$$H = \frac{P^2}{2M} + \sum_{\alpha=1}^{N} \frac{p_\alpha^2}{2m_\alpha} + V(q, x_\alpha) \quad , \tag{11}$$

with the potential

$$V(q, x_\alpha) = V(q) + \frac{1}{2} \sum_{\alpha=1}^{N} m_\alpha w_\alpha^2 (x_\alpha - \frac{c_\alpha}{m_\alpha w_\alpha^2} q)^2 \quad . \tag{12}$$

2.2 Langevin equation from Caldeira-Leggett Hamiltonian

The Hamilton equation

$$\frac{dH}{dq_j} = -\dot{P}_j \tag{13}$$

is applied to the Caldeira-Leggett Hamiltonian, Eq.(10), with the aim of obtaining the equations of motion. The moment is the linear moment whose form is

$$P_j = m\dot{q} \tag{14}$$

where q is the coordinate used for the equation of motion. The Hamilton equation is for the system position coordinate q and for the reservoir positions coordinate x_α. The equation of motion of the position system coordinate is

$$\frac{dH}{dq} = V'(q) + \frac{1}{2} \sum_{\alpha=1}^{N} \frac{d}{dq} \left(-2x_\alpha c_\alpha F(q) + \frac{c_\alpha^2}{m_\alpha w_\alpha^2} F^2(q) \right) = -\dot{P}_j = -M\ddot{q} \quad , \tag{15}$$

and the final form of the equation of motion for the q coordinate is

$$M\ddot{q} + V'(q) + \sum_{\alpha=1}^{N} \frac{c_\alpha^2}{m_\alpha w_\alpha^2} F(q) F'(q) = F'(q) \sum_{\alpha=1}^{N} c_\alpha x_\alpha \quad . \tag{16}$$

The reservoir positions coordinates give as many equations as there are degrees of freedom in the reservoir. All the equations of the reservoir coordinates motion have the same structure and their form come from the Hamilton equation, Eq.(13), as

$$\frac{dH}{dx_\alpha} = \sum_{\alpha=1}^{N} (m_\alpha w_\alpha^2 x_\alpha - c_\alpha F(q)) = -\dot{P}_j = -\sum_{\alpha=1}^{N} m_\alpha \ddot{x}_\alpha \quad . \tag{17}$$

Then, every equation of the reservoir coordinates motion is

$$m_\alpha \ddot{x}_\alpha + m_\alpha w_\alpha^2 x_\alpha = c_\alpha F(q) \quad , \tag{18}$$

where the normalised equation respect to mass is

$$\ddot{x}_\alpha + w_\alpha^2 x_\alpha = \frac{c_\alpha}{m_\alpha} F(q) \quad . \tag{19}$$

There are two types of equation of motion, the associated to the system, Eq.(16), and the associated to the reservoir, Eq.(19). The reservoir equation is a second order differential equation with an inhomogeneous term. First, the homogeneous equation associated

$$\ddot{x}_\alpha + w_\alpha^2 x_\alpha = 0 \tag{20}$$

is solved

$$x_\alpha(t) = a\cos(w_\alpha t) + b\sin(w_\alpha t) \quad , \tag{21}$$

the coefficients a and b depend on the initial conditions of the system, $x_\alpha^{(0)}$ and $p_\alpha^{(0)}$. The coefficient a is

$$a = x_\alpha^{(0)} \tag{22}$$

and it is the a value because if the argument of the cosine is 0, the value of the cosine is 1. For the coefficient b, the position equation is derived

$$\dot{x}_\alpha(t) = -a w_\alpha \sin(w_\alpha t) + b w_\alpha \cos(w_\alpha t) \quad , \tag{23}$$

where at the origin of time the equation is reduced to

$$\dot{x}_\alpha(0) = b w_\alpha \qquad \longrightarrow \qquad b = \frac{p_\alpha^{(0)}}{m_\alpha w_\alpha} \quad . \tag{24}$$

The result for the homogeneous part of Eq.(19) is

$$x_\alpha^{hom} = x_\alpha^{(0)}\cos(w_\alpha t) + \frac{P_\alpha^{(0)}}{m_\alpha w_\alpha}\sin(w_\alpha t) \quad . \tag{25}$$

The inhomogeneous term is solved with the Green function, [11]. The Green's

function in the Eq.(19) is achieved through a Fourier transform and the differential equation with the Green operator is

$$\frac{d^2G(t,t')}{dt^2} + w_\alpha^2 G(t,t') = \frac{1}{m}\delta(t-t') \qquad . \tag{26}$$

The next step is to define the relationship between the Green function space and the reciprocal Green function space. The relationship between two spaces is made with a Fourier transform

$$\tilde{G}(k,t') = \int_{-\infty}^{+\infty} G(t,t')e^{-ikt}dt \qquad , \tag{27}$$

$$G(t,t') = \int_{-\infty}^{+\infty} \tilde{G}(k,t')e^{ikt}dk \qquad . \tag{28}$$

The Green function expressed in reciprocal space applied to the differential equation, Eq.(26), reads

$$[-k^2 + w_\alpha^2]\tilde{G}(k,t') = \frac{e^{-ikt'}}{m_\alpha} \qquad \longrightarrow \qquad \tilde{G}(k,t') = \frac{e^{-ikt'}}{m_\alpha(w_\alpha^2 - k^2)} \qquad . \tag{29}$$

After, the Green's function is represented in initial space with the following expression

$$G(t,t') = \frac{-1}{2\pi m_\alpha}\int_{-\infty}^{+\infty} \frac{e^{ik(t-t')}}{(w_\alpha^2 - k^2)}dk \qquad , \tag{30}$$

this integral is solved with the residue theorem. This integral has two singularities, $k = \pm w_\alpha$, and the integral in the complex plane is

$$G(t,t') = \frac{-1}{2\pi}\int_C \frac{e^{ik(t-t')}}{m_\alpha(k-w_\alpha)(k+w_\alpha)}dk = \frac{-i}{2m_\alpha}(Res[w_\alpha] + Res[-w_\alpha]) \qquad , \tag{31}$$

where the residues for the integral are

$$Res[w_\alpha] = \lim_{k\to w_\alpha}\left[(k-w_\alpha)\frac{e^{ik(t-t')}}{(k-w_\alpha)(k+w_\alpha)}\right] = \lim_{k\to w_\alpha}\left[\frac{e^{ik(t-t')}}{(k+w_\alpha)}\right] = \frac{e^{iw_\alpha(t-t')}}{2w_\alpha} \qquad , \tag{32}$$

$$Res[-w_\alpha] = \lim_{k\to -w_\alpha}\left[(k+w_\alpha)\frac{e^{ik(t-t')}}{(k+w_\alpha)(k-w_\alpha)}\right] = \lim_{k\to -w_\alpha}\left[\frac{e^{ik(t-t')}}{(k-w_\alpha)}\right] = \frac{-e^{-iw_\alpha(t-t')}}{2w_\alpha} \qquad . \tag{33}$$

Then, the Green function is determined as

$$G(t,t') = \frac{-i}{m_\alpha w_\alpha}\left(\frac{e^{iw_\alpha(t-t')} - e^{-iw_\alpha(t-t')}}{2}\right) = \frac{1}{m_\alpha w_\alpha}\sin(w_\alpha(t-t'))H(t-t') \qquad , \tag{34}$$

where $H(t-t')$ is the Heaviside function. The range of the time values is [0,t] with t definite positive and the Green operator reads

$$G(t,t') = \frac{\sin(w_\alpha(t-t'))}{m_\alpha w_\alpha} \quad . \tag{35}$$

The inhomogeneous solution is calculated with the Green function as

$$x^{in}(t) = \int_0^t G(t,t')\frac{F(t')}{m_\alpha}dt' = \int_0^t \frac{\sin(w_\alpha(t-t'))}{m_\alpha w_\alpha}\frac{c_\alpha F(q(t'))}{m_\alpha}dt' \quad . \tag{36}$$

Then, the final expression is

$$x^{in}(t) = \frac{c_\alpha}{m_\alpha w_\alpha}\int_0^t \sin[w_\alpha(t-t')]F[q(t')]dt' \quad . \tag{37}$$

The total position solution is

$$x(t) = x^{hom}(t) + x^{in}(t) = x_\alpha^{(0)}\cos(w_\alpha t) + \frac{p_\alpha^{(0)}}{m_\alpha w_\alpha}\sin(w_\alpha t) + \frac{c_\alpha}{m_\alpha w_\alpha}\int_0^t \sin(w_\alpha(t-t'))F[q(t')]dt' \quad , \tag{38}$$

and this solution is represented in the velocity of the system coordinates instead of the position. The variable change is done by integration by parts

$$\int_0^t dt' \sin(w_\alpha(t-t'))F[q(t')] = \frac{1}{w_\alpha}\left[F[q(t)] - \cos(w_\alpha t)F[q(0)]\right] - \int_0^t dt' \frac{\cos(w_\alpha(t-t'))}{w_\alpha} \quad . \tag{39}$$

The expression of the total position solution, Eq.(38), with the velocity of the system coordinate is

$$\begin{aligned} x(t) = x_\alpha^{(0)}\cos(w_\alpha t) + \frac{p_\alpha^{(0)}}{m_\alpha w_\alpha}\sin(w_\alpha t) + \frac{c_\alpha}{m_\alpha w_\alpha^2}\left[F[q(t)] - \cos(w_\alpha t)F[q(0)]\right] \\ - \frac{c_\alpha}{m_\alpha w_\alpha^2}\int_0^t dt' \cos(w_\alpha(t-t'))F'[q(t')]\dot{q}(t') \end{aligned} \quad . \tag{40}$$

The evolution of the position, Eq.(40), for the motion equation of the reservoir, Eq.(19), is inserted in the motion equation of the system, Eq.(16).

$$\begin{aligned} M\ddot{q} + V'(q) + \sum_{\alpha=1}^N \frac{c_\alpha^2}{m_\alpha w_\alpha^2}F(q)F'(q) = F'(q)\sum_{\alpha=1}^N c_\alpha \Bigg[x_\alpha^{(0)}\cos(w_\alpha t) + \frac{p_\alpha^{(0)}}{m_\alpha w_\alpha}\sin(w_\alpha t) + \\ + \frac{c_\alpha}{m_\alpha w_\alpha^2}\left[F[q(t)] - \cos(w_\alpha t)F[q(0)]\right] - \frac{c_\alpha}{m_\alpha w_\alpha^2}\int_0^t dt' \cos(w_\alpha(t-t'))F'[q(t')]\dot{q}(t')\Bigg] \end{aligned} \quad , \tag{41}$$

this equation can be simplified as

$$\begin{aligned} M\ddot{q}+\sum_{\alpha=1}^{N}\frac{c_\alpha^2}{m_\alpha w_\alpha^2}F'(q)\left[\cos(w_\alpha t)F[q(0)]+\int_0^t dt'\cos(w_\alpha(t-t'))F'[q(t')]\dot{q}(t')\right] \\ +V'(q)=F'(q)\sum_{\alpha=1}^{N}c_\alpha\left[x_\alpha^{(0)}\cos(w_\alpha t)+\frac{p_\alpha^{(0)}}{m_\alpha w_\alpha}\sin(w_\alpha t)\right] \quad . \end{aligned} \tag{42}$$

At this point, two new variables are introduced, the memory friction kernel and the force. The mathematical description of these variables is [1]

$$\gamma(t-t')=H(t-t')\frac{1}{M}\sum_{\alpha}\frac{c_\alpha^2}{m_\alpha w_\alpha^2}\cos(w_\alpha(t-t')) \quad , \tag{43}$$

$$\zeta(t)=\sum_{\alpha=1}^{N}c_\alpha\left[x_\alpha^{(0)}\cos(w_\alpha t)+\frac{p_\alpha^{(0)}}{m_\alpha w_\alpha}\sin(w_\alpha t)\right] \quad . \tag{44}$$

The motion equation with these variables is

$$M\ddot{q}+V'(q)+F'(q(t))M\int_0^t dt'\gamma(t-t')F'[q(t')]\dot{q}(t')=F'(q)\zeta(t)-MF'[q(t')]F[q(0)]\gamma(t) \quad . \tag{45}$$

With the initial values $x_\alpha^{(0)}$ and $p_\alpha^{(0)}$ for the unperturbed reservoir ($F(q)=0$), the canonical classical equilibrium density at time origin is [1]

$$\rho_R^{(0)}=Z^{-1}e^{-\beta H(0)}=Z^{-1}e^{-\beta\sum_\alpha(\frac{p_\alpha^{(0)2}}{2m_\alpha}+\frac{m_\alpha w_\alpha^2}{2}x_\alpha^{(0)2})} \quad . \tag{46}$$

The force $\zeta(t)$ is defined as a fluctuating force with colored noise and Gaussian statistical properties

$$\langle\zeta(t)\rangle_{\rho_R^{(0)}}=0 \qquad \langle\zeta(t)\zeta(t')\rangle_{\rho_R^{(0)}}=Mk_BT\gamma(t-t') \quad , \tag{47}$$

where the second relationship is the fluctuation dissipation theorem.

The motion equation for a generalized force, Eq.(45), is restricted for the linear force ($F(q)=q$) and the motion equation is reduced to

$$M\ddot{q}+V'(q)+M\int_0^t dt'\gamma(t-t')\dot{q}(t')=\zeta(t)-M\gamma(t)q(0) \quad . \tag{48}$$

The stochastic motion equation does not match with the usual form of the Langevin equation because there is an extra term, $-M\gamma(t)q(0)$. Then, a variable change reads

$$\xi(t) = \zeta(t) - M\gamma(t)q(0) \qquad . \tag{49}$$

The new force $\xi(t)$ does not disappear on average when it is taken respect to the density defined in Eq.(46). The force $\xi(t)$ is treated like a random Gaussian force and for this purpose the canonical equilibrium density must consider the contribution associated with the force

$$\rho_R = Z^{-1} e^{-\beta \sum_\alpha \left(\frac{p_\alpha^{(0)2}}{2m_\alpha} + \frac{m_\alpha w_\alpha^2}{2} (x_\alpha^{(0)} - \frac{c_\alpha}{m_\alpha w_\alpha^2} q(0))^2 \right)} \qquad , \tag{50}$$

where the statistical properties of the random force with the new canonical equilibrium density are

$$\langle \xi(t) \rangle_{\rho_R} = 0 \qquad \langle \xi(t)\xi(t') \rangle_{\rho_R} = 2Mk_BT\gamma(t-t') \qquad . \tag{51}$$

The new force applied to the motion equation gives the standard form of the generalized Langevin equation

$$M\ddot{q} + V'(q) + M \int_0^t dt' \gamma(t-t')\dot{q}(t') = \xi(t) \qquad . \tag{52}$$

2.3 Langevin equation to Schrödinger-Langevin equation

The standard Langevin equation is the classical equation of motion for particles. The next step is to obtain the Schrödinger equation associated with the standard Langevin equation of motion whose name is the Schrödinger-Langevin equation. It is an equation with a remarkable non linear character. This section is separated in the three ways to link the two equations: Kostin procedure, the generalization of the Kostin procedure and Nottale scale relativity method.

2.3.1 Kostin procedure

The first development between these two equations was carried out by Kostin in [3]. It was developed by a heuristic method and it requires Heisenberg operators. The

Heisenberg momentum operator reads

$$P = M\dot{X} \qquad , \tag{53}$$

where X as the Heisenberg operator for q. The Langevin equation Eq.(52) in function of the Heisenberg momentum operator is

$$\dot{P} = -\alpha P - V'(X) + \xi(t) \qquad , \tag{54}$$

with

$$\alpha = \int_0^t dt' \gamma(t - t') \qquad . \tag{55}$$

This Langevin equation in function of the averages values is

$$\langle \dot{P} \rangle = -\alpha \langle P \rangle - \langle V'(X) \rangle + \langle \xi(t) \rangle \qquad . \tag{56}$$

The purpose of this development is the Schrödinger equation to this system. For it, the most generalized Scrödinger equation is

$$i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2M} \frac{d\psi^2}{dx^2} + \left[V(x) + V_R(x,t) + V_d \right] \psi(x,t) \qquad , \tag{57}$$

where the different potentials are $V(x)$ for the system potential, $V_R(x,t)$ for the random force and V_d for the friction term.

The relationship with the Langevin equation comes from the average value of the momentum. In Schrödinger theory, the average value for the momentum is the self adjoint scalar product as

$$\langle P(t) \rangle = (\psi(t), P\psi(t)) \qquad , \tag{58}$$

and for the time derivative of the average momentum is

$$\frac{d\langle P(t) \rangle}{dt} = \left(\frac{d\psi(t)}{dt}, P\psi(t) \right) + \left(\psi, P(\frac{d\psi}{dt}) \right) \qquad . \tag{59}$$

Then, with the Schrödinger equation, Eq.(57), and the momentum operator as

$$P = -i\hbar\frac{d}{dx} \quad , \tag{60}$$

the time derivative of the average momentum is

$$\frac{d\langle P(t)\rangle}{dt} = -\langle\frac{dV}{dx}\rangle - \langle\frac{dV_R}{dx}\rangle - \langle\frac{dV_d}{dx}\rangle \quad . \tag{61}$$

The average momentum can be defined as

$$\langle\dot{P}\rangle = \frac{d\langle P\rangle}{dt} \tag{62}$$

and it relates the Langevin equation of the Heisenberg momentum operator Eq.(56) to the potentials of the Schrödinger equation. The averages potentials are

$$\langle\frac{dV}{dx}\rangle = \langle V'(X)\rangle \qquad \langle\frac{dV_R}{dx}\rangle = -\langle\xi(t)\rangle \qquad \langle\frac{dV_d}{dx}\rangle = \alpha\langle P\rangle \quad . \tag{63}$$

The values of the system potential and the random potentials are easy to obtain and the potentials read

$$V = V(X) \qquad V_R = -x\xi(t) \quad . \tag{64}$$

The friction potential requires the average momentum in function of the position. For it, the scalar product of the average momentum Eq.(58) with the self adjoint property and the momentum in the position coordinate Eq.(60) gives

$$\langle P\rangle = \int \frac{-i\hbar}{2}\left[\frac{d\psi}{dx}\psi^* - \psi\frac{d\psi^*}{dx}\right]dx \quad . \tag{65}$$

This average momentum is introduced in the equation to determine the friction potential Eq.(63) as

$$\langle\frac{dV_d}{dx}\rangle = \int \psi^*\frac{dV_d}{dx}\psi dx = \alpha\int \frac{-i\hbar}{2}\left[\frac{d\psi}{dx}\psi^* - \psi\frac{d\psi^*}{dx}\right]dx \tag{66}$$

and it is reduced to

$$\frac{dV_d}{dx} = \frac{-i\alpha\hbar}{2}\left[\frac{1}{\psi}\frac{d\psi}{dx} - \frac{1}{\psi^*}\frac{d\psi^*}{dx}\right] \quad . \tag{67}$$

The right term is better expressed in function of the logarithm with the property [6]

$$\nabla \ln(\psi) = \frac{\nabla \psi}{\psi} \tag{68}$$

and the derivative of the friction potential is

$$\frac{dV_d}{dx} = \frac{-i\alpha\hbar}{2} \frac{d}{dx} \left(\ln(\psi) - \ln(\psi^*) \right) \quad . \tag{69}$$

Then, the friction potential by integration is

$$V_d = \frac{-i\alpha\hbar}{2} \ln\left(\frac{\psi}{\psi^*}\right) + W(t) \quad . \tag{70}$$

$W(t)$ is a constant integration that represents the time dependence of the potential in the position derivative. The value can be determined with the expected value of mechanic energy. The mechanic energy of this system has the kinetic energy and the potential energy with the system potential and the random potential. The average energy in function of the kinetic and potentials is

$$\langle E(t) \rangle = \frac{\langle P^2 \rangle}{2M} + \langle V(t) \rangle + \langle V_R(t) \rangle \quad . \tag{71}$$

This average energy is also determined by the wave function and it reads

$$\langle E(t) \rangle = i\hbar \int \psi^* \frac{d\psi}{dx} dx \quad , \tag{72}$$

with the Schrödinger equation, Eq.(57), reads

$$\langle E(t) \rangle = \int \psi^* \left[-\frac{\hbar^2}{2M} \frac{d^2}{dx^2} + V(x) + V_R(x,t) + V_d \right] \psi dx \quad . \tag{73}$$

The average of the square momentum operator Eq.(60) is

$$\langle P^2 \rangle = -\hbar^2 \int \psi^* \frac{d^2}{dx^2} \psi dx \tag{74}$$

and if it is introduced in the average energy the equation gives the kinetic energy. The three other contributions correspond to the potentials and the friction potential is not considered at the initial average energy Eq.(71) and this contribution is the value of

$W(t)$. Then, the friction average energy is

$$W(t) = -\int \psi^* V_d \psi dx = \frac{i\alpha\hbar}{2}\left\langle \ln\left(\frac{\psi}{\psi^*}\right)\right\rangle \quad . \tag{75}$$

The development of the Schrödinger-Langevin equation is fullfilled because the different contributions of the Langevin motion equation are introduced as potentials in the Schrödinger equation. The Schrödinger-Langevin equation is

$$i\hbar\frac{d\psi}{dt} = -\frac{\hbar^2}{2M}\frac{d\psi^2}{dx^2} + \left[V(x) - x\xi(t) - \frac{i\alpha\hbar}{2}\left(\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle \ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right)\right]\psi(x,t) \quad , \tag{76}$$

2.3.2 Generalization of the Kostin procedure

This generalization considers the general form of the Schrödinger equation with a number of unknown contributions to the potential. This development is a generalization because it does not need the Heisenberg operators. These unknown potentials are intended to be related to the different terms of the standard Langevin equation, Eq.(52). With this consideration, the Schrödinger equation is [4]

$$i\hbar\frac{d\psi}{dt} = \left[\frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2 + V(x) + V_d + V_r\right]\psi \quad . \tag{77}$$

The unknown potentials considered are a dissipative potential, V_d, and a random potential, V_r. The heuristic method defines these potentials as a function of the terms of the standard Langevin equation. For this purpose, the standard Langevin equation, Eq.(52), is expressed as a function of the mean value of the components

$$M\langle\ddot{q}\rangle + \langle V'(x)\rangle + M\alpha\langle\dot{q}(t')\rangle = \langle\xi(t)\rangle \quad . \tag{78}$$

where α is from Eq.(55). If this equation is compared to the classical definition of the force reads

$$\langle F\rangle = M\langle\ddot{q}\rangle = -\langle V'(x)\rangle - M\int_0^t dt'\gamma(t-t')\langle\dot{q}(t')\rangle + \langle\xi(t)\rangle \quad , \tag{79}$$

with the force determined as

$$F = -\frac{dV}{dx} \quad . \tag{80}$$

The potentials of the Schrödinger equation, Eq.(88), are related with their contributions to the equation of motion. The potential of the system, $V(x)$, generates the force $V'(x)$ and its proof is trivial. The dissipative contribution is associated with the velocity of the coordinate

$$\langle -\frac{dV_d}{dx} \rangle = -M\alpha \langle \dot{q} \rangle \quad . \tag{81}$$

The average value of the velocity is written as a function of the probability current. For that, it is necessary to define the probability current

$$J = \frac{-i\hbar}{2M} \left[\psi^* \frac{d}{dx}\psi - \psi \frac{d}{dx}\psi^* \right] \quad . \tag{82}$$

The relationship between the average value of velocity and the probability current is developed in the appendix.6.1 and the final relationship is

$$\frac{d}{dt}\langle x \rangle = \int J dx \quad . \tag{83}$$

Then, this expression is introduced in the dissipative potential, Eq.(81), and expressed in integral form

$$\int \psi^* \left(-\frac{dV_d}{dx} \right) \psi dx = -M\alpha \int J dx \quad . \tag{84}$$

It results in a functional expression of the dissipative potential in terms of the wave function [4]

$$V_d = M\alpha \int \frac{J}{\psi\psi^*} dx \quad . \tag{85}$$

The random potential is considered with the random force of the motion equation

$$\langle -\frac{dV_r}{dx} \rangle = \langle \xi(t) \rangle \quad , \tag{86}$$

and the final expression for the random potential is

$$V_r = -x\xi(t) \quad . \tag{87}$$

After the dissipative potential, Eq.(85), and the random potential, Eq.(87), are

established, the undetermined Schrödinger equation, Eq.(88), can be expressed as the standard Schrödinger-Langevin equation

$$i\hbar\frac{d\psi}{dt} = \left[\frac{1}{2m}(-i\hbar\frac{d}{dx})^2 + V(x) + M\alpha\int\frac{J}{\psi\psi^*}dx - x\xi(t) + W(t)\right]\psi \quad , \tag{88}$$

with an extra term that does not depend on positions

$$W(t) = - < V_d > \quad . \tag{89}$$

This term can not be added before because only depends on time, and not in positions. It is associated with the conservation of the total density probability along time. The description of $W(t)$ is known because in the Kostin procedure comes from considering the average energy, but in this generalization it does not make sense. In the generalization, the definition of the dissipative force is different because it is defined as a function of the probability current and not as a function the logarithm of the wave function.

In order to verify this, the dissipative term of Eq.(88) is expanded with the probability current of Eq.(82) as

$$M\alpha\int\frac{J}{\psi\psi^*}dx = \frac{-i\hbar\alpha}{2}\int\frac{[\psi^*\nabla\psi - \psi\nabla\psi^*]}{\psi\psi^*}dx = \frac{-i\hbar\alpha}{2}\int\left[\frac{\nabla\psi}{\psi} - \frac{\nabla\psi^*}{\psi^*}\right]dx \quad , \tag{90}$$

with the property for the gradient of a logarithm, Eq.(68), reads

$$\begin{aligned}\frac{-i\hbar\alpha}{2}\int\left[\frac{\nabla\psi}{\psi} - \frac{\nabla\psi^*}{\psi^*}\right]dx &= \frac{-i\hbar\alpha}{2}\int\left[\nabla\ln(\psi) - \nabla\ln(\psi^*)\right]dx = \\ =\frac{-i\hbar\alpha}{2}\ln(\psi) - \ln(\psi^*) &= \frac{-i\hbar\alpha}{2}\ln\left(\frac{\psi}{\psi^*}\right) \quad ,\end{aligned} \tag{91}$$

where the definition in function of the logarithm of the wave function is the same of the Kostin procedure. Furthermore, if the $W(t)$ term is defined in the same way as in the Kostin procedure, the generalization gives the same Schrödinger-Langevin equation, Eq.(76), as in the Kostin procedure.

2.3.3 Scale relativity method

The scale relativity method was developed by Laurent Nottale. This theory exposes a fractal space-time that is not visible in the classical regime, but it is visible in the

quantum regime. This fractal space-time allow non differential trajectories, characteristic of the quantum regime. At this point, the quantum regime can be separated into a differential part and in a non differential part. The fractal dimension for the quantum regime is $D_F = 2$ while for the classical regime it is $D_F = 1$.[5]

This difference between the two regimes is related to leaving complex velocity and covariant derivative of time instead of the classical derivative of time. The covariant derivative of time needs to consider that the fractal dimension is 2 and it causes second order terms to be introduced. It is done with a Taylor expansion, where the first order includes a gradient (first order derivative) while the second order involves a Laplacian (second order derivative).[5] In the second order an imaginary unit from the complex velocity is added. The general expression for the covariant time derivative of order two is

$$\frac{D}{Dt} = \frac{d}{dt} + V * \nabla - i\mathcal{D}\Delta \qquad . \tag{92}$$

This section applies the scale relativity to the standard Langevin equation, Eq.(52). The first step is to consider the covariant derivative for the acceleration expressed in velocity terms[6]

$$M\left[\frac{d}{dt}\dot{q} + (\dot{q} * \nabla)\dot{q} - i\mathcal{D}\nabla\dot{q}\right] + V'(q) + M\int_0^t dt'\gamma(t-t')\dot{q}(t') = \xi(t) \qquad . \tag{93}$$

The relationship between the velocity and the coordinate is

$$\dot{q} = \frac{\nabla q}{M} \qquad , \tag{94}$$

where the mass terms oppose the velocity. The equation of motion with the velocity reads

$$M\left[\frac{d}{dt}\frac{\nabla q}{M} + (\frac{\nabla q}{M} * \nabla)\frac{\nabla q}{M} - i\mathcal{D}\Delta\frac{\nabla q}{M}\right] + V'(q) + M\int_0^t dt'\gamma(t-t')\frac{\nabla q(t')}{M} = \xi(t) \qquad . \tag{95}$$

For the integration of this equation, all terms are written as a function of the gradient.[6] For this purpose, the following identity for gradients, so useful in fluid mechanics, is applied for the velocity

$$(\nabla q * \nabla)\nabla q = \nabla\left(\frac{(\nabla q)^2}{2}\right) - \nabla q \times (\nabla \times \nabla q) \qquad , \tag{96}$$

where the second part is the rotational for a gradient, which is 0 by the equality of the cross derivatives. Then, the identity can be reduced as

$$(\nabla q * \nabla)\nabla q = \nabla \frac{(\nabla q)^2}{2} \quad . \tag{97}$$

With it, the motion equation, Eq.(95), reads

$$\nabla \frac{d}{dt} q + \nabla \frac{(\nabla q)^2}{2M} - i\mathcal{D}\nabla\Delta q + \nabla V(q) + \nabla \alpha q - \nabla \int \xi(t) d\vec{r} = 0 \quad , \tag{98}$$

whose integration is

$$\frac{d}{dt} q + \frac{(\nabla q)^2}{2M} - i\mathcal{D}\Delta q + V(q) + \alpha q - \int \xi(t) d\vec{r} + W(t) = 0 \quad . \tag{99}$$

The term $W(t)$ is added because it is a constant integration independent of position and has non zero value when dissipation effects are considered. The integration of the random force is simplified because the force does not depend on position and the system is considered along one axis. The integration is

$$\int \xi(t) d\vec{r} = x\xi(t) \quad . \tag{100}$$

The next step is a Cole-Hopf transformation [6] in order to write the equation as a function of the wave function and not as a function of the coordinate q. The Cole-Hopf transformation is

$$q = -2iM\mathcal{D}\ln(\psi) \quad , \tag{101}$$

with the diffusion variable defined as [6]

$$\mathcal{D} = \frac{\hbar}{2M} \quad , \tag{102}$$

where $\hbar$ is the Planck constant introduced by the quantum regime. It must be inversely proportional to the mass because in the classical world quantum effects are not seen. The factor 2 is added by the Taylor expansion performed for the time covariant derivative.

Then, the Cole-Hopf transformation, Eq.(101), with the diffusion coefficient, Eq.(102), is introduced in the equation obtained after integration into the motion equation,

Eq.(99). The resultant equation is

$$\frac{d}{dt}(-i\hbar\ln(\psi))+\frac{(\nabla(-i\hbar\ln(\psi)))^2}{2M}-i\frac{\hbar}{2M}\Delta(-i\hbar\ln(\psi))+V+\alpha(-i\hbar\ln(\psi))-x\xi(t)+W(t)=0 \tag{103}$$

and can be simplified with the following properties of the gradient Eq.(68) and Laplacian for a logarithm [6]

$$\Delta\ln(\psi)=\frac{\Delta\psi}{\psi}-\frac{1}{\psi^2}(\nabla\psi)^2 \quad . \tag{104}$$

The simplified equation is a Schrödinger equation

$$i\hbar\frac{d}{dt}\psi=\left[-\frac{\hbar^2}{2M}\Delta+V-i\hbar\alpha\ln(\psi)-x\xi(t)+W(t)\right]\psi \quad . \tag{105}$$

The possibility of complex variables specific to the quantum regime makes it necessary to decompose the friction component, α, into $\alpha=\alpha_R+i\alpha_I$. A restriction of the dissipation component is necessary to the realisation of the local conservation of the probability density function. The change is to consider only the real part of the dissipative force with the relationship

$$-i\hbar Re\left[\alpha\ln(\psi)\right]=\hbar Im\left[\alpha\ln(\psi)\right] \quad , \tag{106}$$

which is applied to the friction coefficient as

$$Im\left[\alpha\ln(\psi)\right]=\alpha_I\ln|\psi|-\frac{1}{2}i\alpha_R\ln\left(\frac{\psi}{\psi^*}\right) \quad . \tag{107}$$

The Schrödinger equation, Eq.(105), with the friction coefficient separated into real and imaginary is

$$i\hbar\frac{d}{dt}\psi=\left[-\frac{\hbar^2}{2M}\Delta+V+\hbar\alpha_I\ln|\psi|-\frac{\hbar}{2}i\alpha_R\ln\left(\frac{\psi}{\psi^*}\right)-x\xi(t)+W(t)\right]\psi \quad . \tag{108}$$

Previously, the integration term, $W(t)$, was defined as a term that is non zero when there are dissipation effects. It appears by definition as a function of the average value of the real friction coefficient. Then, the expression of this term is

$$W(t)=\frac{\hbar}{2}i\alpha_R\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle \quad . \tag{109}$$

With this definition, the Schrödinger equation reads

$$i\hbar\frac{d}{dt}\psi = \left[-\frac{\hbar^2}{2M}\Delta + V + \hbar\alpha_I \ln|\psi| - \frac{\hbar}{2}i\alpha_R\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle \ln\left\langle\frac{\psi}{\psi^*}\right\rangle\right\rangle\right] - x\xi(t)\right]\psi \quad , \tag{110}$$

and it becomes in the Schrödinger-Langevin equation when only real frictions are considered, $\alpha_I = 0$ [12]. The standard Schrödinger-Langevin equation reads

$$i\hbar\frac{d}{dt}\psi = \left[-\frac{\hbar^2}{2M}\Delta + V - \frac{\hbar}{2}i\alpha_R\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle \ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right] - x\xi(t)\right]\psi \quad . \tag{111}$$

It can be seen how the Kostin procedure (heuristic method) and the scale relativity method give the same Schrödinger-Lagevin equation at the end.

3 Brownian-Bohmian quantum motion

After the Schrödinger-Langevin equation, Eq.(111), is obtained it is applied to study the Brownian- Bohmian motion for a Gaussian wave packet and for a stretched Gaussian wave packet. For this purpose, the wave function is represented in the polar or Bohm form [12, 13, 9]

$$\psi(r,t) = |\psi(r,t)|e^{\frac{iS(r,t)}{\hbar}} \quad . \tag{112}$$

This wave function is introduced in the Scrödinger-Langevin equation by means of the chain rule. The various derivatives needed to represent the equation in the Bohm form are

$$\frac{d\psi}{dt} = \frac{d|\psi(r,t)|}{dt}e^{\frac{iS(r,t)}{\hbar}} + \frac{i}{\hbar}\frac{dS(r,t)}{dt}|\psi(r,t)|e^{\frac{iS(r,t)}{\hbar}} \quad , \tag{113}$$

$$\begin{aligned}\nabla^2\psi = \nabla\left[\nabla|\psi(r,t)|e^{\frac{iS(r,t)}{\hbar}} + \frac{i}{\hbar}\nabla S(r,t)e^{\frac{iS(r,t)}{\hbar}}\right] = \\ \left[\nabla^2|\psi(r,t)| + \frac{2i}{\hbar}\nabla S(r,t)\nabla|\psi(r,t)| - \frac{(\nabla S(r,t))^2}{\hbar^2}|\psi(r,t)|\right]e^{\frac{iS(r,t)}{\hbar}}\end{aligned} \quad , \tag{114}$$

$$\frac{\psi}{\psi^*} = \frac{|\psi(r,t)|e^{\frac{iS(r,t)}{\hbar}}}{|\psi(r,t)|e^{\frac{-iS(r,t)}{\hbar}}} = e^{\frac{2iS(r,t)}{\hbar}} \quad . \tag{115}$$

With the above, the Scrödinger-Langevin equation, Eq.(111), is written in the Bohm form, Eq.(112), as

$$i\hbar\frac{d|\psi(r,t)|}{dt}e^{\frac{iS(r,t)}{\hbar}} - \frac{dS(r,t)}{dt}|\psi(r,t)|e^{\frac{iS(r,t)}{\hbar}} = -\frac{\hbar^2}{2M}\nabla^2|\psi(r,t)|e^{\frac{iS(r,t)}{\hbar}} + [V - x\xi(t)]\,\psi$$
$$-\frac{i\hbar}{M}\nabla S(r,t)\nabla|\psi(r,t)|e^{\frac{iS(r,t)}{\hbar}} + \frac{(\nabla S(r,t))^2}{2M}|\psi(r,t)|e^{\frac{iS(r,t)}{\hbar}} + \alpha_R\left[S(r,t) - \langle S(r,t)\rangle\right] \tag{116}$$

and it can be separated into two equations, one for the real terms and other for the imaginary terms of the equation. The two equations are

$$\begin{cases} -\dfrac{dS(r,t)}{dt} = -\dfrac{\hbar^2}{2M}\dfrac{\nabla^2|\psi(r,t)|}{|\psi(r,t)|} + \dfrac{(\nabla S(r,t))^2}{2M} + \alpha_R\left[S(r,t) - \langle S(r,t)\rangle\right] + [V - x\xi(t)] \\ i\hbar\dfrac{d|\psi(r,t)|}{dt}e^{\frac{iS(r,t)}{\hbar}} = -\dfrac{i\hbar}{M}\nabla S(r,t)\nabla|\psi(r,t)|e^{\frac{iS(r,t)}{\hbar}} \end{cases} \tag{117}$$

The imaginary equation multiplying both components by the conjugate wave function reads

$$\frac{d|\psi(r,t)|^2}{dt} + \frac{\nabla S(r,t)}{M}\nabla|\psi(r,t)|^2 = 0 \qquad . \tag{118}$$

Then, the velocity field is defined in a similar way as Eq.(94) and the density operator is also introduced

$$v(r,t) = \frac{\nabla S(r,t)}{M} \qquad , \tag{119}$$

$$\rho(r,t) = |\psi(r,t)|^2 \qquad . \tag{120}$$

With these two variable changes the set of two equations are [12]

$$\begin{cases} -\dfrac{dS(r,t)}{dt} = -\dfrac{\hbar^2}{2M}\dfrac{\nabla^2|\psi(r,t)|}{|\psi(r,t)|} + \dfrac{(\nabla S(r,t))^2}{2M} + \alpha_R\left[S(r,t) - \langle S(r,t)\rangle\right] + [V - x\xi(t)] \\ \dfrac{d\rho(r,t)}{dt} + \nabla(\rho(r,t)v(r,t)) = 0 \end{cases} \tag{121}$$

The second equation is the well-known continuity equation, and the first equation is the modified Hamilton-Jacobi equation with a quantum potential and a dissipative term. The quantum potential is [12]

$$Q = -\frac{\hbar^2}{2M}\frac{\nabla^2|\psi(r,t)|}{|\psi(r,t)|} \qquad . \tag{122}$$

This potential is a key concept in the Bohm interpretation of quantum mechanics as it is said in the introduction.

After that, a space derivative is introduced into the modified Hamilton-Jacobi equation which gives

$$\nabla\frac{dS(r,t)}{dt}+\nabla\frac{(\nabla S(r,t))^2}{2M}=-\nabla\left[V-x\xi(t)+Q\right]-\alpha_R\nabla S(r,t) \quad , \tag{123}$$

with the property for the gradient of Eq.(97) reads

$$\frac{d\nabla S(r,t)}{dt}+\left(\frac{\nabla S(r,t)}{M}*\nabla\right)\nabla S(r,t)=-\nabla\left[V-x\xi(t)+Q\right]-\alpha_R\nabla S(r,t) \quad . \tag{124}$$

Then, the velocity field, Eq.(119), is introduced into the previous equation as[12]

$$\left(\frac{d}{dt}+v(r,t)*\nabla\right)v(r,t)=-\frac{1}{M}\nabla\left[V-x\xi(t)+Q\right]-\alpha_R v(r,t) \quad . \tag{125}$$

This equation is a better way of expressing the evolution of the dynamics of the quantum system for the Brownian quantum motion than the modified Hamilton-Jacobi equation because it depends on the velocity field.

The set of equations in Eq.(121) gives the evolution of the system considered. The system is described by the form of the wave packet density (Gaussian wave packet or stretched Gaussian wave packet). From this point on, the study of the different wave packets will be treated separately and for only one space dimension.

3.1 Gaussian wave packet

The density operator, Eq.(120), of a Gaussian wave packet reads [12, 13, 9]

$$\rho(x,t)=\frac{1}{\sqrt{2\pi}\sigma(t)}e^{\frac{-(x-q(t))^2}{2\sigma^2(t)}} \quad , \tag{126}$$

where the modulus of the wave function is defined as the square root of the density operator

$$|\psi(x,t)|=\frac{1}{\sqrt{\sqrt{2\pi}\sigma(t)}}e^{\frac{-(x-q(t))^2}{4\sigma^2(t)}} \quad . \tag{127}$$

The velocity field of the Gaussian wave packet is defined by the continuity equation,

Eq.(121). For this purpose, the time derivative of the density operator is

$$\frac{d\rho(x,t)}{dt} = \frac{1}{\sqrt{2\pi}\sigma(t)}\left[\frac{4(x-q(t))\sigma(t)^2\dot{q}(t) + 4\sigma(t)\dot{\sigma}(t)(x-q(t))^2}{4\sigma(t)^4}\right] e^{\frac{-(x-q(t))^2}{2\sigma(t)^2}} \quad , \tag{128}$$

and its application in the continuity equation gives

$$\rho(x,t)v(x,t) = -\int dx\rho(x,t)\frac{(x-q(t))}{\sigma(t)^2}\left[\dot{q}(t) + \frac{\dot{\sigma}(t)}{\sigma(t)}(x-q(t))\right] \quad , \tag{129}$$

where the part outside the brackets agrees with the space derivative of the Gaussian wave packet. The velocity field is given by the integration as [12, 13, 9]

$$v(x,t) = \dot{q}(t) + \frac{\dot{\sigma}(t)}{\sigma(t)}(x-q(t)) \quad . \tag{130}$$

With the velocity field and the modulus of the wave packet, the purpose is the representation of the motion equation as a function of the Gaussian variables (position and width). Then, the velocity field, Eq.(130), and the quantum potential, Eq.(122), are introduced for the Gaussian wave packet in the motion equation, Eq.(125).

The derivatives of the velocity in the motion equation for the Gaussian wave packet are

$$\frac{dv}{dt} = \ddot{q}(t) + \frac{\ddot{\sigma}(t)}{\sigma(t)}(x-q(t)) - \frac{\dot{\sigma}(t)^2}{\sigma(t)^2}(x-q(t)) - \frac{\dot{\sigma}(t)}{\sigma(t)}\dot{q} \quad , \tag{131}$$

$$v\frac{dv}{dx} = \frac{\dot{\sigma}(t)^2}{\sigma(t)^2}(x-q(t)) + \frac{\dot{\sigma}(t)}{\sigma(t)}\dot{q} \quad . \tag{132}$$

The quantum potential for the Gaussian wave packet is

$$\frac{d^2}{dx^2}|\psi(x,t)| = \frac{1}{2\sigma(t)^2}|\psi(x,t)|\left[\frac{(x-q(t))^2}{2\sigma(t)^2} - 1\right] \quad , \tag{133}$$

$$Q = \frac{-\hbar^2(x-q(t))^2}{8M\sigma(t)^4} \quad . \tag{134}$$

These velocity derivatives and the quantum potential are introduced in the motion equation. After that, the equation is divided in terms of the dependence of the trajectories as

$$(x-q(t))\left[\ddot{\sigma}(t) + \alpha_R\dot{\sigma}(t) - \frac{\hbar^2}{4M^2\sigma(t)^3}\right] + (x-q(t))^0\sigma(t)\left[\ddot{q}(t) + \alpha_R\dot{q}(t) + \frac{1}{M}\nabla(V(x) - x\xi(t))\right] = 0 \quad . \tag{135}$$

Now, the wave packet approximation is considered, which implies that the potential changes very slowly around the classical trajectory $q(t)$. With this approximation, a first order Taylor expansion for the potential is realized [12, 13, 9]

$$\frac{dV}{dx} = \frac{dV}{dx}\Big|_{x=q(t)} + \frac{d^2V}{dx^2}\Big|_{x=q(t)} (x - q(t)) \quad . \tag{136}$$

With it, the equation follows

$$\begin{aligned} &(x - q(t)) \left[\ddot{\sigma}(t) + \alpha_R \dot{\sigma}(t) - \frac{\hbar^2}{4M^2\sigma(t)^3} + \frac{\sigma(t)}{M}\frac{d^2V}{dx^2}\Big|_{x=q(t)}\right] \\ &+(x - q(t))^0 \sigma(t) \left[\ddot{q}(t) + \alpha_R \dot{q}(t) + \frac{1}{M}\frac{dV}{dx}\Big|_{x=q(t)} - \frac{\xi(t)}{M}\right] = 0 \end{aligned} \quad . \tag{137}$$

The decoupling of the center position and the width of the wave packet is applied taking into account the linear independence between the terms. Thus, there are two separate equations [12, 13, 9]

$$\ddot{q}(t) + \alpha_R \dot{q}(t) + \frac{1}{M}\frac{dV}{dx}\Big|_{x=q(t)} = \frac{\xi(t)}{M} \quad , \tag{138}$$

$$\ddot{\sigma}(t) + \alpha_R \dot{\sigma(t)} - \frac{\hbar^2}{4M^2\sigma(t)^3} + \frac{\sigma(t)}{M}\frac{d^2V}{dx^2}\Big|_{x=q(t)} = 0 \quad . \tag{139}$$

The center of the wave packet evolution is described with the Langevin equation, Eq.(52), where the friction coefficient is defined in Eq.(55). The width evolution is a type of equation known as damped Pinney equation.

3.2 Stretched Gaussian wave packet

The probability density for the stretched Gaussian wave packet is

$$\rho(x,t) = \frac{1}{\sqrt{2\pi(1+\eta^2)}\sigma(t)} e^{\frac{-(x-q(t))^2}{2\sigma^2(t)(1+\eta^2)}} \quad , \tag{140}$$

and the modulus of the wave function associated to this probability density is

$$|\psi(x,t)| = \frac{1}{\sqrt{\sqrt{2\pi(1+\eta^2)}\sigma(t)}} e^{\frac{-(x-q(t))^2}{4\sigma^2(t)(1+\eta^2)}} \quad . \tag{141}$$

Following the same scheme as the Gaussian wave packet, the velocity field of the

wave packet is established by the continuity equation, Eq.(121). Previously, the time derivative of the probability density reads

$$\frac{d\rho(x,t)}{dt} = -\frac{e^{\frac{-(x-q(t))^2}{2\sigma(t)^2(1+\eta^2)}}}{\sqrt{2\pi(1+\eta^2)}\sigma(t)}\left[\frac{-4(x-q(t))\sigma(t)^2(1+\eta^2)\dot{q}(t) - 4\sigma(t)\dot{\sigma}(t)(1+\eta^2)(x-q(t))^2}{4\sigma(t)^4(1+\eta^2)^2}\right] , \tag{142}$$

and the continuity equation associated is

$$\rho(x,t)v(x,t) = -\int dx\rho(x,t)\frac{(x-q(t))}{\sigma(t)^2(1+\eta^2)}\left[\dot{q}(t) + \frac{\dot{\sigma}(t)}{\sigma(t)}(x-q(t))\right] \quad . \tag{143}$$

The velocity field of this equation gives the same velocity field as that obtained for the Gaussian wave packet, Eq.(130). The derivatives for the velocity field with this wave packet were defined in Eq.(131) and Ec.(132) in the previous section 3.1 for the Gaussian wave packet. The quantum potential, Ec.(122), for this wave packet reads

$$\frac{d^2}{dx^2}|\psi(x,t)| = \frac{|\psi(x,t)|}{2\sigma(t)^2(1+\eta^2)}\left[\frac{(x-q(t))^2}{2\sigma(t)^2(1+\eta^2)} - 1\right] \quad , \tag{144}$$

$$Q = -\frac{\hbar^2(x-q(t))^2}{8M\sigma(t)^4(1+\eta^2)^2} \quad . \tag{145}$$

With these derivatives and this quantum potential, the motion equation, Eq.(125), for the stretched Gaussian wave packet reads

$$\begin{aligned}(x-q(t))\left[\ddot{\sigma}(t) + \alpha_R\dot{\sigma(t)} - \frac{\hbar^2}{4M^2\sigma(t)^3(1+\eta^2)^2}\right] \\ +(x-q(t))^0\sigma(t)\left[\ddot{q}(t) + \alpha_R\dot{q}(t) + \frac{1}{M}\nabla(V(x) - x\xi(t))\right] = 0 \quad .\end{aligned} \tag{146}$$

The wave packet approximation gets a first order Taylor expansion for the potential as Eq.(136) by the same reason as the Gaussian wave packet. After that, the equation is separated into a center position equation and in a width equation by the linear dependence between the different powers of the trajectory, with the same procedure as the Gaussian wave packet. Then, the set of equations is as follows

$$\ddot{q}(t) + \alpha_R\dot{q}(t) + \frac{1}{M}\frac{dV}{dx}\Big|_{x=q(t)} = \frac{\xi(t)}{M} \quad , \tag{147}$$

$$\ddot{\sigma}(t) + \alpha_R\dot{\sigma(t)} - \frac{\hbar^2}{4M^2\sigma^3(1+\eta^2)^2} + \frac{\sigma(t)}{M}\frac{d^2V}{dx^2}\Big|_{x=q(t)} = 0 \quad . \tag{148}$$

The set of equations is similar to that obtained for the Gaussian wave packet, in that the only difference is in the term associated with the quantum potential for the width equation. The difference does not change the structure of the equations, the position equation is a Langevin equation, Eq.(52), while for the width is a damped Pinney equation.

The position equation is unchanged because the only difference between both wave packets are in the width with the stretching factor $1+\eta^2$. This factor perturbs the quantum potential and it generates the difference between the evolution of the width in the two types of wave packets. The stretched Gaussian wave packet recovers in the wave packet and in the width equation the Gaussian wave packet if η is 0.

3.3 Free particle

The free particle assumes that there is not potential, $V(x)=0$. For this, the Langevin position equation for both wave packets in this work is

$$\ddot{q}(t)+\alpha_R\dot{q}(t)=\frac{\xi(t)}{M} \quad , \tag{149}$$

while for the width the Gaussian equation and the stretched Gaussian equation are

$$\begin{cases} \ddot{\sigma}(t)+\alpha_R\dot{\sigma(t)}-\dfrac{\hbar^2}{4M^2\sigma(t)^3}=0 \\ \ddot{\sigma}(t)+\alpha_R\dot{\sigma(t)}-\dfrac{\hbar^2}{4M^2\sigma(t)^3(1+\eta^2)^2}=0 \end{cases} . \tag{150}$$

The Langevin position equation, Eq.(149), is an inhomogeneous second order differential equation and it can be considered as a first order if it is expressed in function of the velocity. The equation expressed as a function of the velocity of the transformed space reads

$$(s\dot{q}(s)-\dot{q}(0))+\alpha_R\dot{q}(s)=\frac{\xi(t)}{M}\longrightarrow\dot{q}(s)=\frac{\dot{q}(0)}{s+\alpha_R}+\frac{\xi(t)}{M(s+\alpha_R)} \quad , \tag{151}$$

and the solution requires an inverse Laplace transform of $1/(s+\alpha_R)$ which value is

$exp(-\alpha_R t)$ [14]. The velocity is

$$\dot{q}(t) = \dot{q}(0)e^{-\alpha_R t} + \frac{1}{M}\int_0^t d\tau \xi(\tau) e^{-\alpha_R(t-\tau)} \quad , \tag{152}$$

and the position evolution by integration is

$$q(t) = q(0) + \dot{q}(0)\frac{1}{\alpha_R}(1 - e^{-\alpha_R t}) + \frac{1}{M\alpha_R}\int_0^t d\tau \xi(\tau) e^{-\alpha_R(t-\tau)} \quad . \tag{153}$$

The average values of the positions and velocities are separated in the deterministic term and in the stochastic term where it is applied the properties of Eq.(51). The general structure for this decomposition is

$$\langle a \rangle = a_d + \langle a_s \rangle \quad . \tag{154}$$

The average position and velocity only has deterministic term by the properties of the stochastic force, Eq.(51), which is Gaussian statistics. These averages are

$$\langle q(t) \rangle = q(0) + \dot{q}(0)\frac{1}{\alpha_R}(1 - e^{-\alpha_R t}) \quad , \tag{155}$$

$$\langle \dot{q}(t) \rangle = \dot{q}(0)e^{-\alpha_R t} \quad . \tag{156}$$

The average squared position and the average squared speed have a stochastic term. First, the stochastic component for the average squared position is

$$\langle q_s(t)^2 \rangle = \langle \frac{1}{M^2\alpha_R^2}\int_0^t dt' \left[1 - e^{-\alpha_R(t-t')}\right] \int_{-t'}^{t-t'} d\tau \xi(t')\xi(\tau) \left[1 - e^{-\alpha_R(t-t'-\tau)}\right] \rangle \quad , \tag{157}$$

where the average only affects for the random force with the value defined in Eq.(51). Then, the average square position is

$$\begin{aligned} \langle q_s(t)^2 \rangle = \frac{2k_B T}{M\alpha_R}\int_0^t dt' \left[1 - e^{-\alpha_R(t-t')}\right] \int_{-t'}^{t-t'} d\tau \left[1 - e^{-\alpha_R(t-t'-\tau)}\right] \delta(t'-\tau) = \\ = \frac{2k_B T}{M\alpha_R}\int_0^t dt' \left[1 - e^{-\alpha_R(t-t')}\right]^2 \quad . \end{aligned} \tag{158}$$

This integral gives the following average squared position for the stochastic component

$$\langle q_s(t)^2\rangle = \frac{2k_BT}{M\alpha_R^2}\left[\alpha_R t - \frac{3}{2} + 2e^{-\alpha_R t} - \frac{1}{2}e^{-2\alpha_R t}\right] \quad . \tag{159}$$

For the average squared velocity the mathematical calculation is

$$\begin{aligned}\langle \dot{q}_s(t)^2\rangle &= \langle \frac{1}{M^2}\int_0^t d\tau \int_0^t d\tau' \xi(\tau)\xi(\tau') e^{-\alpha_R(2t-\tau-\tau')}\rangle = \\ &= \frac{e^{-2\alpha_R t}}{M^2}\int_0^t d\tau \int_0^t d\tau' \langle \xi(\tau)\xi(\tau')\rangle e^{\alpha_R(\tau+\tau')} \quad ,\end{aligned} \tag{160}$$

with the properties of Eq.(51) it becomes

$$\begin{aligned}\langle \dot{q}_s(t)^2\rangle &= \frac{2k_BT\alpha_R e^{-2\alpha_R t}}{M}\int_0^t d\tau \int_0^t d\tau' \delta(\tau'-\tau) e^{\alpha_R(\tau+\tau')} = \\ &= \frac{2k_BT\alpha_R e^{-2\alpha_R t}}{M}\int_0^t d\tau e^{2\alpha_R\tau} = \frac{k_BT}{M}(1-e^{-2\alpha_R t}) \quad .\end{aligned} \tag{161}$$

Then, the average squared position and the average squared velocity are

$$\langle q(t)^2\rangle = \left(q(0) + \dot{q}(0)\frac{1}{\alpha_R}(1-e^{-\alpha_R t})\right)^2 - \frac{k_BT}{M\alpha_R^2}(3+e^{-2\alpha_R t}-4e^{-\alpha_R t}-2\alpha_R t) \quad , \tag{162}$$

$$\langle \dot{q}(t)^2\rangle = \dot{q}(0)^2 e^{-2\alpha_R t} + \frac{k_BT}{M}(1-e^{-2\alpha_R t}) \quad . \tag{163}$$

The following calculation is another average over the initial velocities, $\dot{q}(0) = 0$, respect to the initial average described before, giving a double average. For it, the average initial values of the velocity are defined as

$$\langle \dot{q}(0)\rangle = 0 \quad , \tag{164}$$

$$\langle \dot{q}(0)^2\rangle = \frac{k_BT}{M} \quad . \tag{165}$$

With these initial conditions, the double averages for positions and velocities are

$$\langle\langle q(t)\rangle\rangle = q(0) \quad , \tag{166}$$

$$\langle\langle \dot{q}(t)\rangle\rangle = 0 \quad , \tag{167}$$

$$\langle\langle q(t)^2\rangle\rangle = q(0)^2 + \frac{2k_BT}{M\alpha_R}(t - \frac{1-e^{-\alpha_R t}}{\alpha_R}) \quad , \tag{168}$$

$$\langle\langle \dot{q}(t)^2 \rangle\rangle = \frac{k_B T}{M} \quad . \tag{169}$$

3.3.1 Diffusion coefficient

The diffusion coefficient is defined in Einstein's relation as [12]

$$D = \frac{k_B T}{M \alpha_R} \quad . \tag{170}$$

The diffusion coefficient at long times ($t >> \alpha_R^{-1}$) is related with the mean square displacement for a one dimensional motion as

$$\langle (q(t) - q(0))^2 \rangle \simeq 2Dt \quad , \tag{171}$$

where the mean squared displacement is considered as Eq.(168) the Einstein's relation is accomplished. The classical time dependent diffusion coefficient reads

$$D_{cl}(t) = \frac{k_B T}{M \alpha_R} (1 - \frac{1 - e^{-\alpha_R t}}{\alpha_R t}) \quad . \tag{172}$$

The mean squared displacement can be determined from the Bohmian stochastic trajectories. First, the Bohmian stochastic trajectories are obtained from an integration of the velocity field, Eq.(130). The Bohmian stochastic trajectories are

$$x(x^{(0)}, t) = q(t) + \frac{\sigma(t)}{\sigma(0)} (x^{(0)} - q(0)) \quad . \tag{173}$$

The difference between this function and the initial conditions is

$$x(x^{(0)}, t) - x^{(0)} = q(t) - q(0) + \left(\frac{\sigma(t)}{\sigma(0)} - 1 \right) (x^{(0)} - q(0)) \quad . \tag{174}$$

Then, the double average of the mean squared displacement with initial conditions is

$$\langle\langle (x(x^{(0)}, t) - x^{(0)})^2 \rangle\rangle = \langle\langle (q(t) - q(0))^2 \rangle\rangle + 2\langle\langle (q(t) - q(0)) \rangle\rangle \left(\frac{\sigma(t)}{\sigma(0)} - 1 \right) (x^{(0)} - q(0)) + \left(\frac{\sigma(t)}{\sigma(0)} - 1 \right)^2 (x^{(0)} - q(0))^2 \quad . \tag{175}$$

After that, it is necessary to obtain the diffusion coefficient an average over the possible initial values of the Bohmian position

$$\overline{\langle\langle(x(x^{(0)},t)-x^{(0)})^2\rangle\rangle} = \int dx^{(0)}\rho(x^{(0)},0)\langle\langle(x(x^{(0)},t)-x^{(0)})^2\rangle\rangle \quad . \tag{176}$$

The initial distribution used is the stretched Gaussian wave packet, Eq.(140), because the Gaussian distribution can be recovered with the stretching factor equal to 0. The double average value of the position defined in Eq.(168). It is considered the double average of Eq.(166) for the linear term that becomes null.

$$\overline{\langle\langle(x(x^{(0)},t)-x^{(0)})^2\rangle\rangle} = \int dx^{(0)} \frac{\frac{2k_BT}{M\alpha_R}(t-\frac{1-e^{-\alpha_R t}}{\alpha_R}) + \left(\frac{\sigma(t)}{\sigma(0)}-1\right)^2 (x^{(0)}-q(0))^2}{\sqrt{2\pi(1+\eta^2)}\sigma(0)} e^{-\frac{(x^{(0)}-q(0))^2}{2\sigma(0)^2(1+\eta^2)}} \quad . \tag{177}$$

The integration of this equation needs a change of variable determined as $u = x^{(0)} - q(0)$ and the following Gaussian integrals

$$\int dx e^{-\frac{x^2}{2a}} = \sqrt{\frac{2\pi}{a}} \qquad \int dx x^2 e^{-\frac{x^2}{2a}} = \sqrt{\frac{2\pi}{a}}\frac{1}{a} \tag{178}$$

Then, the mean squared displacement of the Bohmian stochastic trajectories with the stretched Gaussian wave packet is

$$\overline{\langle\langle(x(x^{(0)},t)-x^{(0)})^2\rangle\rangle} = \frac{2k_BT}{M\alpha_R}(t-\frac{1-e^{-\alpha_R t}}{\alpha_R}) + (\sigma(t)-\sigma(0))^2(1+\eta^2) \quad . \tag{179}$$

The diffusion coefficient defined with the mean squared displacement, Eq.(171), and with the resulting classical diffusion coefficient, Eq.(172), are compared. The Gaussian wave packet is shown in the first equation and for the stretched Gaussian wave packet is the second equation.

$$\begin{cases} D_q(t) = D_{cl}(t) + \dfrac{1}{2t}(\sigma(t)-\sigma(0))^2 \\ D_q(t) = D_{cl}(t) + \dfrac{1}{2t}(\sigma(t)-\sigma(0))^2(1+\eta^2) \end{cases} \quad . \tag{180}$$

The result shows that the diffusion coefficient of Bohmian trajectories defined as quantum diffusion has an extra term dependent on the width of the wave function. This extra term can disappear if the width does not change with time, where the quantum diffusion coefficient recovers the classical diffusion coefficient form.

Another way to find the value of the diffusion coefficient is with the velocity autocorrelation function [14]. It starts with the velocity function, Eq.(152), and the equation is changed to be defined as a function of the velocity autocorrelation function

$$\langle \dot{q}(0)\dot{q}(t)\rangle = \langle \dot{q}(0)^2\rangle e^{-\alpha_R t} + \frac{1}{M}\int_0^t d\tau \langle \dot{q}(0)\xi(\tau)\rangle e^{-\alpha_R(t-\tau)} \quad , \tag{181}$$

where the second term is 0 because the two variables are not correlated. The first term requires the mean squared velocity, Eq.(169), and the velocity autocorrelation function reads

$$\langle \dot{q}(0)\dot{q}(t)\rangle = \frac{k_B T}{M} e^{-\alpha_R t} \quad . \tag{182}$$

The diffusion coefficient is determined by time integration of the velocity autocorrelation function [12]

$$D = \int_0^{+\infty} dt \langle \dot{q}(0)\dot{q}(t)\rangle = \frac{k_B T}{M\alpha_R} \quad . \tag{183}$$

The Einstein relation is recovered with the velocity autocorrelation function.

3.3.2 Uncertainty product

The uncertainty product gives a measure of the evolution of the system. The operators required for the uncertainty product are the position and momentum operators and their squares. The development is with the stretched Gaussian wave packet, Eq.(140), because it is a generalization of the Gaussian wave packet, Eq.(126), which it can be recovered with the stretching factor equals to 0.

The position and momentum operators are calculated with the first Gaussian integral considered in Eq.(178) and read [12]

$$\overline{\hat{x}} = \int dx x \rho(x,t) = \int dx \frac{x}{\sqrt{2\pi(1+\eta^2)}\sigma(t)} e^{-\frac{(x-q(t))^2}{2\sigma(t)^2(1+\eta^2)}} = q(t) \quad , \tag{184}$$

$$\overline{\hat{p}} = -i\hbar \int dx \psi^* \frac{d}{dx}\psi = -i\hbar \int dx \left[\frac{(x-q(t))}{\sigma(t)^2(1+\eta^2)} + \frac{i}{\hbar}\frac{dS}{dx}\right]\rho(x,t) \quad . \tag{185}$$

The action $S(x,t)$ is related to the two different definitions of the velocity field, Eq.(130)

and Eq.(119), and the momentum operator applied for this is

$$\overline{\hat{p}} = \int dx \left[\frac{-i\hbar(x-q(t))}{\sigma(t)^2(1+\eta^2)} + M[\dot{q}(t) + \frac{\dot{\sigma}(t)}{\sigma(t)}(x-q(t))] \right] \frac{e^{-\frac{(x-q(t))^2}{2\sigma(t)^2(1+\eta^2)}}}{\sqrt{2\pi(1+\eta^2)\sigma(t)^2}} \quad . \tag{186}$$

With a variable change as $u = x - q(t)$ and the integration of an odd power multiplied by an exponential is 0 and the first Gaussian integral, Eq.(178), gives

$$\overline{\hat{p}} = M\dot{q}(t) \quad . \tag{187}$$

The squared position operator is

$$\begin{aligned} \overline{\hat{x}}^2 &= \int dx x^2 \rho(x,t) = \int dx \frac{x^2}{\sqrt{2\pi(1+\eta^2)}\sigma(t)} e^{-\frac{(x-q(t))^2}{2\sigma(t)^2(1+\eta^2)}} = \\ &= \int dx \frac{(u+q(t))^2}{\sqrt{2\pi(1+\eta^2)}\sigma(t)} e^{-\frac{(u)^2}{2\sigma(t)^2(1+\eta^2)}} \quad , \end{aligned} \tag{188}$$

and the squared position operator with the Gaussian integrals, Eq.(178), follows

$$\overline{\hat{x}}^2 = q(t)^2 + \sigma(t)^2(1+\eta^2) \quad . \tag{189}$$

The squared momentum operator is

$$\overline{\hat{p}}^2 = \hbar^2 \int dx \left| \frac{d\psi}{dx} \right|^2 = \hbar^2 \int dx \left[\frac{-(x-q(t))}{2\sigma(t)^2(1+\eta^2)} + \frac{i}{\hbar} \left(\frac{dS}{dx} \right) \right]^2 \rho(x,t) \quad . \tag{190}$$

The velocity field is introduced from the action, Eq.(119), with the velocity field, Eq.(130). Then, the absolute value operator is

$$\overline{\hat{p}}^2 = \int dx \left[\frac{\hbar^2(x-q(t))^2}{4\sigma(t)^4(1+\eta^2)^2} + M^2 \left(\dot{q}(t)^2 + 2\frac{\dot{q(t)}\dot{\sigma}(t)}{\sigma(t)}(x-q(t)) + \frac{\dot{\sigma}(t)^2}{\sigma(t)^2}(x-q(t))^2 \right) \right] \rho(x,t) \quad . \tag{191}$$

The integral with the correspondent variable change $u = x - q(t)$, with the Gaussian integrals, Eq.(178), and with value of the integral 0 for odd powers multiplying. Then, the squared momentum operator is

$$\overline{\hat{p}}^2 = \frac{\hbar^2}{4\sigma(t)^2(1+\eta^2)} + M^2\dot{q}^2 + M^2\dot{\sigma}(t)^2(1+\eta^2) \quad . \tag{192}$$

The next step is the double average of the variances of the position and momentum

with the operators, Eqs.(184,187,189,192). [12]

$$(\langle\langle\Delta x\rangle\rangle)^2 = \langle\langle\bar{\hat{x}}^2\rangle\rangle - \langle\langle\bar{\hat{x}}\rangle\rangle^2 = \langle\langle q(t)^2\rangle\rangle - \langle\langle q(t)\rangle\rangle^2 + \sigma(t)^2(1+\eta^2) \quad , \tag{193}$$

$$(\langle\langle\Delta p\rangle\rangle)^2 = \langle\langle\bar{\hat{p}}^2\rangle\rangle - \langle\langle\bar{\hat{p}}\rangle\rangle^2 = M^2\left(\langle\langle\dot{q}(t)^2\rangle\rangle - \langle\langle\dot{q}(t)\rangle\rangle^2 + \dot{\sigma}(t)^2(1+\eta^2)\right) + \frac{\hbar^2}{4\sigma(t)^2(1+\eta^2)} \quad , \tag{194}$$

and it is expressed better with the average relations, Eqs.(166,167,168,169)

$$(\langle\langle\Delta x\rangle\rangle)^2 = \frac{2k_BT}{M\alpha_R}(t - \frac{1-e^{-\alpha_R t}}{\alpha_R}) + \sigma(t)^2(1+\eta^2) \quad , \tag{195}$$

$$(\langle\langle\Delta p\rangle\rangle)^2 = k_BTM + M^2\dot{\sigma}(t)^2(1+\eta^2) + \frac{\hbar^2}{4\sigma(t)^2(1+\eta^2)} \quad . \tag{196}$$

The uncertainty product is defined as [12]

$$U(t) = \sqrt{(\langle\langle\Delta x\rangle\rangle)^2(\langle\langle\Delta p\rangle\rangle)^2} \quad , \tag{197}$$

which for the Brownian motion in a stretched Gaussian distribution is

$$U(t)^2 = \frac{\hbar^2}{4} + M^2\sigma(t)^2\dot{\sigma}(t)^2(1+\eta^2)^2 + \frac{2(k_BT)^2}{\alpha_R}(t - \frac{1-e^{-\alpha_R t}}{\alpha_R}) \\ +k_BT\left[M\sigma(t)^2(1+\eta^2) + \frac{2}{M\alpha_R}(t - \frac{1-e^{-\alpha_R t}}{\alpha_R})\left(M^2\dot{\sigma}(t)^2(1+\eta^2) + \frac{\hbar^2}{4\sigma(t)^2(1+\eta^2)}\right)\right] \quad , \tag{198}$$

while for a Gaussian distribution is

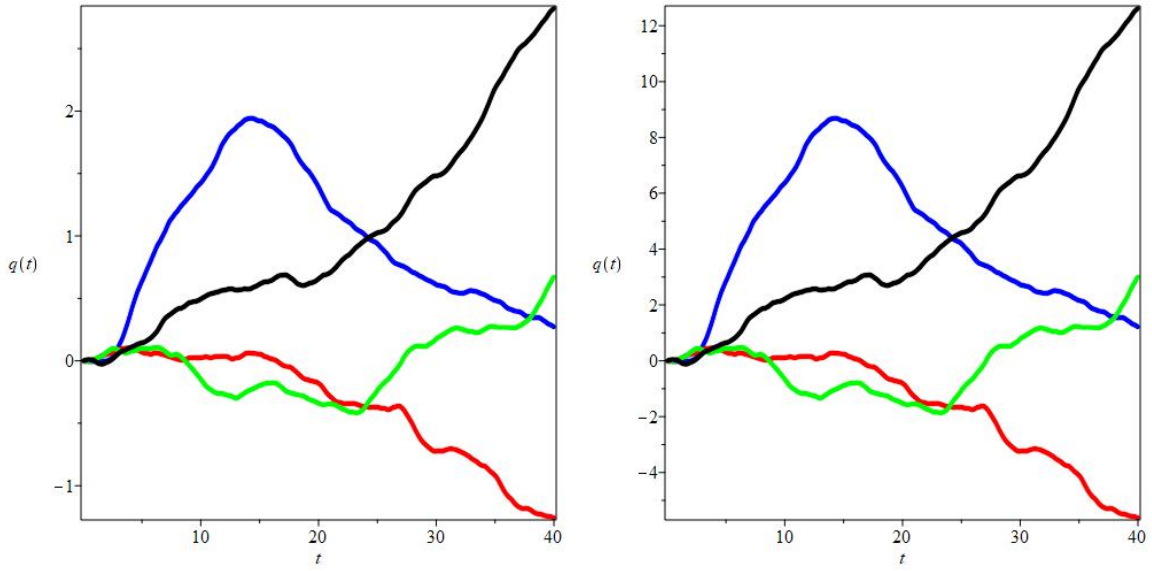
$$U(t)^2 = \frac{\hbar^2}{4} + M^2\sigma(t)^2\dot{\sigma}(t)^2 + \frac{2(k_BT)^2}{\alpha_R}(t - \frac{1-e^{-\alpha_R t}}{\alpha_R}) \\ +k_BT\left[M\sigma(t)^2 + \frac{2}{M\alpha_R}(t - \frac{1-e^{-\alpha_R t}}{\alpha_R})\left(M^2\dot{\sigma}(t)^2 + \frac{\hbar^2}{4\sigma(t)^2}\right)\right] \quad . \tag{199}$$

There is a minimum constant with the same value as the minimum Heisenberg uncertainty value , $U = \frac{\hbar}{2}$, for both types of wave packets . The result without random force and width change corresponds with a minimum uncertainty wave packet regardless the stretching factor.

4 Results

The Brownian-Bohmian motion is described for the Gaussian wave packet and the stretched Gaussian wave packet with the Bohmian stochastic trajectories, the mean squared displacement, the diffusion coefficient and the uncertainty product. The numerical calculations have been done with natural units ($\hbar = 1, M = 1$).

The system evolves according to the Langevin equation, Eq.(149), for the two types of wave packets. The Langevin equation is solved by applying the algorithm proposed in [15] where the random force is considered with random values whose mean value is 0. The initial conditions for the algorithm are $q(0) = 0$ and $\dot{q}(0) = 0$. The number of steps of the algorithm is 4000, the number of stochastic trajectories considered are 4 and the total time evolution is 40. The Langevin equation evolution, Fig.1, shows a different evolution for each stochastic trajectory with a random local evolution generating a random evolution in each trajectory. The temperature changes the intensity of the motion along the coordinate, but the evolution over time is analogous.

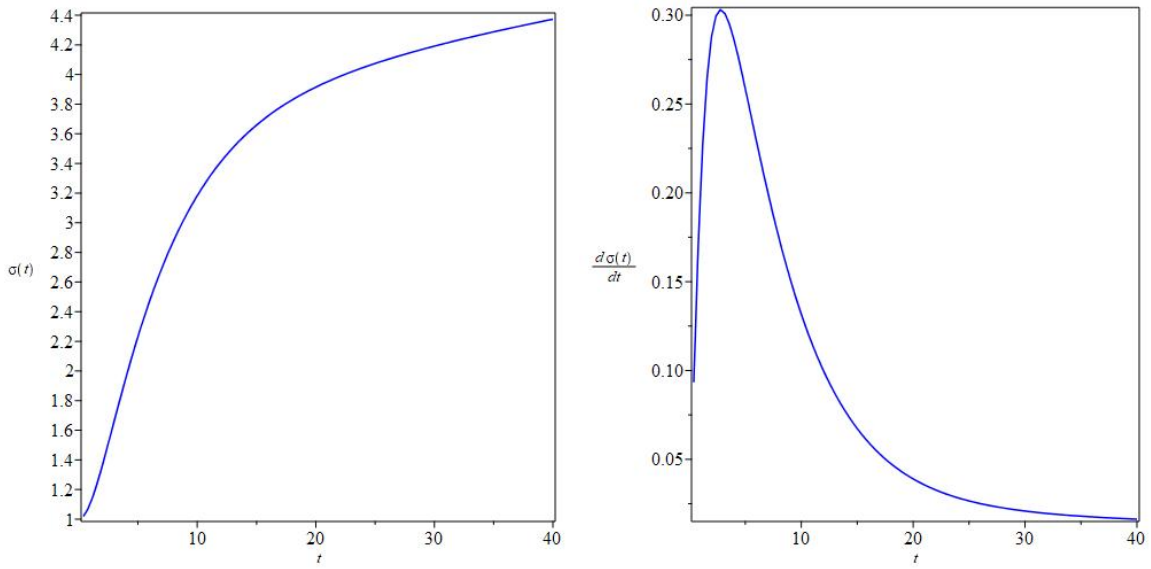


(a) $k_B T = 0.01$. (b) $k_B T = 0.2$.

Figure 1: Langevin equation evolution for four stochastic trajectories with algorithm [15] considering 4000 steps and the equation variables $\alpha_R = 0.2$, the random force $k_B T = 0.01$ and $k_B T = 0.2$ and the initial values $q(0) = 0$ and $\dot{q}(0) = 0$.

The width evolution has been solved in MAPLE with the initial conditions $\sigma(0) = 1$ and $\dot{\sigma}(0) = 0$, considered at the same value as [13]. The time evolution of the width and its derivative is shown in Fig.2 only for the Gaussian wave packet. The width

always grows and it tends to a asymptotically value at infinite time.



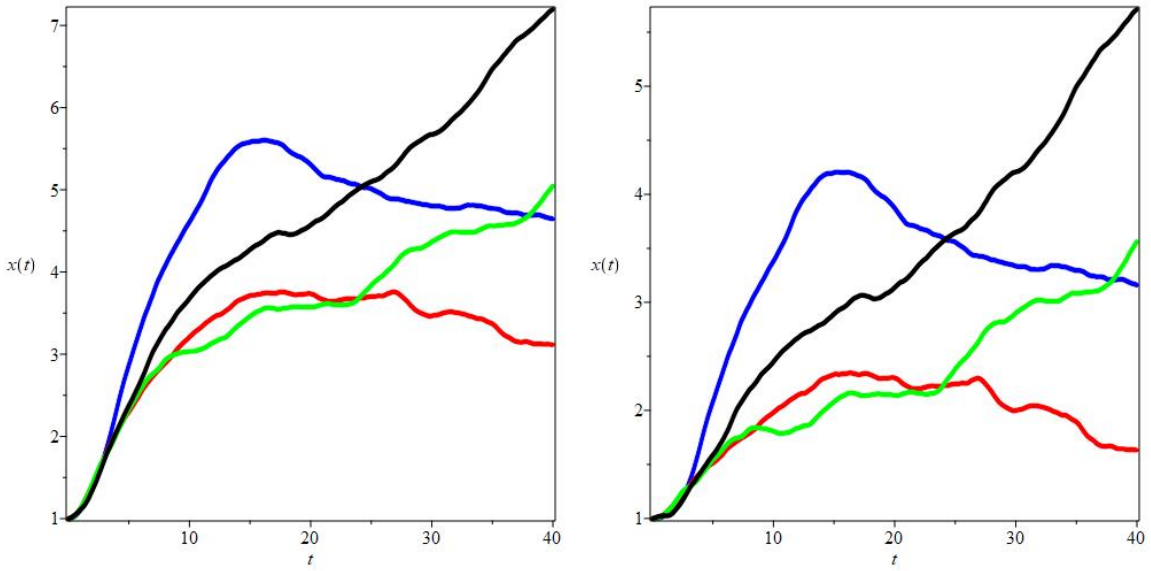
(a) Width. (b) Width derivative.

Figure 2: The time evolution of the Gaussian wave packet for the width and for its derivative with the initial conditions as $\sigma(0) = 1$ and $\dot{\sigma}(0) = 0$. The friction coefficient is $\alpha_R = 0.2$.

The Bohmian stochastic trajectories, Eq.(173), have a contribution to the centre of the wave packet solved by the Langevin equation and a contribution to the width solved by the undamped Pinney equation. The initial position of the Bohmian stochastic trajectory is $x^{(0)} = 1$. Bohmian stochastic trajectories are realized for two temperatures, $k_B T = 0.01$ in Fig.3 and $k_B T = 0.2$ in Fig.4 where the Gaussian wave packet and the stretched Gaussian wave packet are considered. The two wave packets have an analogous evolution, but the Gaussian wave packet has higher trajectories values than the stretched Gaussian wave packet as it can be seen in the end of the black or the red stochastic trajectories. The stochastic trajectories has a random behaviour influenced by the stochastic force and it implies every stochastic trajectory is different from the others.

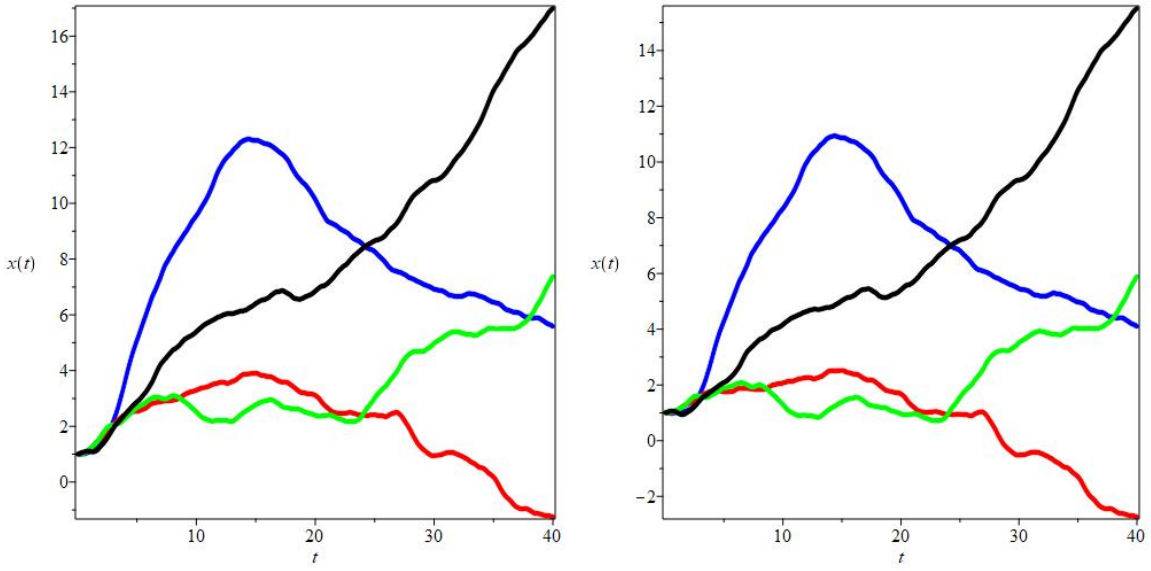
The influence of the stochastic force with the temperature is a greater randomness over time for every stochastic trajectory and a greater difference from the width evolution, which is the evolution for the trajectories without stochastic force.

The random behaviour of each Bohmian stochastic trajectory implies this variable as a bad way to analyze the Brownian-Bohmian quantum motion. Then, the Brownian-Bohmian quantum motion is studied with averaged variables. In particular, with



(a) Gaussian wave packet (b) Stretched Gaussian wave packet.

Figure 3: Bohmian stochastic trajectories with $\alpha_R = 0.2$, $k_B T = 0.01$ and $x^{(0)} = 1$ for a Gaussian wave packet and a stretched Gaussian wave packet with $\eta = 1$. The number of Bohmian stochastic trajectories are four.



(a) Gaussian wave packet (b) Stretched Gaussian wave packet.

Figure 4: Bohmian stochastic trajectories with $\alpha_R = 0.2$, $k_B T = 0.2$ and $x^{(0)} = 1$ for a Gaussian wave packet and a stretched Gaussian wave packet with $\eta = 1$. The number of Bohmian stochastic trajectories are four.

the mean squared displacement, the diffusion coefficient and the uncertainty product defined in the section 3.3. At this point, the Gaussian wave packet and stretched Gaussian wave packet are considered separately.

4.1 Gaussian wave packet

The mean squared displacement and the diffusion coefficient have been considered with two different temperatures, $k_BT = 0.2$ and $k_BT = 0.5$, and with a friction coefficient, $\alpha_R = 0.2$, for their classical and quantum description. The results for the Gaussian wave packet are the same as those obtained in [13].

The mean squared displacement in its quantum framework is Eq.(179) with the stretching factor as 0 and in the classical framework without the width term. The mean squared displacement is plotted in Fig.5. The result shows that the mean squared displacement always grows with time. The quantum regime is greater than the classical regime and both increase with the temperature, but not the difference between them. After the initial time, the mean squared displacement seems linear and the slope depends on the temperature. The dependence on time agrees with the characteristic of the Brownian motion.

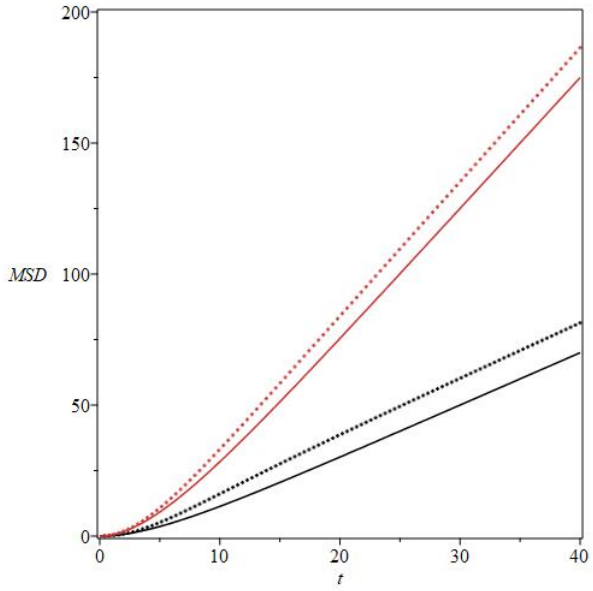


Figure 5: The mean squared displacement for the quantum values are the dotted curves and for the classical values are the solid curves. The red curves are for $k_BT = 0.5$ and the black curves for $k_BT = 0.2$. The friction coefficient is $\alpha_R = 0.2$.

The diffusion coefficient for the quantum regime, Eq.(180), and for the classical regime, Eq.(172). The diffusion coefficient is represented in Fig.6. The diffusion value grows with time until asymptotic times are reached, where the value is constant as predicted by Einstein relation. Temperature increases the quantum and classical diffusion coefficient as their asymptotic values. For the same temperature, the quantum

coefficient diffusion is bigger than the classical one over the whole time and the quantum asymptotic values are slightly larger than the classical one. It implies that the quantum contribution does not disappear with time.

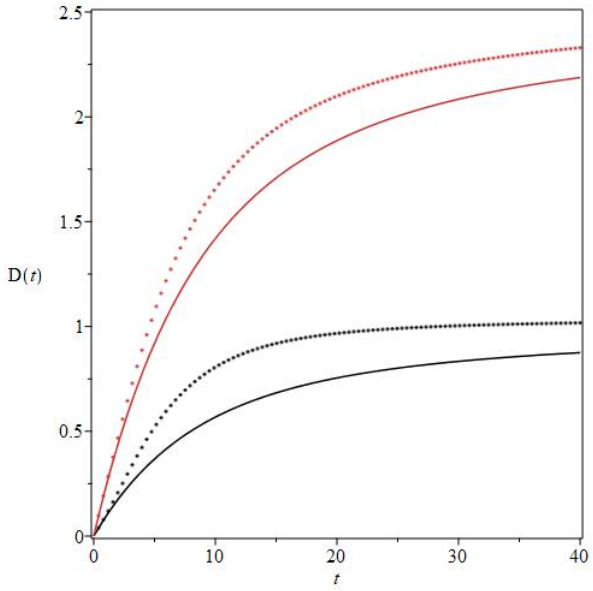
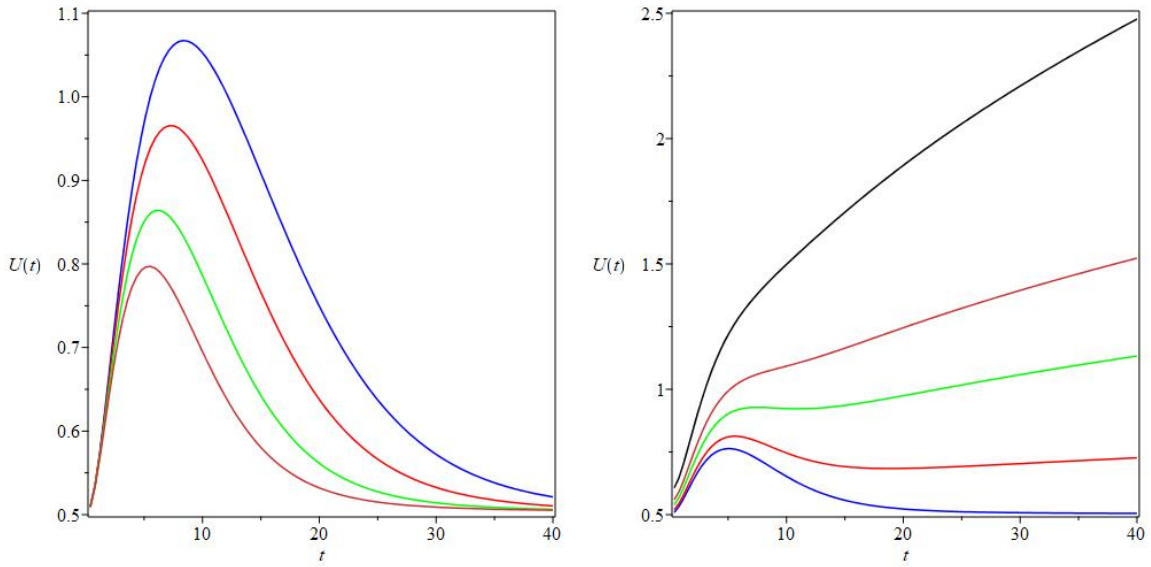


Figure 6: The diffusion coefficient for the quantum values are the dotted curves and for the classical values are the solid curves. The red curves are for $k_BT = 0.5$ and the black curves for $k_BT = 0.2$. The friction coefficient is $\alpha_R = 0.2$.

In the uncertainty product, two different studies are realized. One for the temperature and one for the friction coefficient. Both studies follow the evolution of Eq.(199) and both studies are represented in Fig.7. The minimum value in the graphics is 0.5, in line with the Heisenberg minimum uncertainty product.

Without the random force dependence, $k_BT = 0$, the uncertainty product is ruled by the width derivative as the similar time evolution in a initial growth and a decrease after the maximum value to the asymptotic value at infinite time. For the uncertainty product, the asymptotic value is obtained when the width derivative reaches 0. The higher friction coefficient reduces the maximum value and is achieved earlier. The higher friction coefficient lowers the asymptotic value, but it is still greater than 0.5.

The influence of the temperature obtains a growth at all times without an asymptotic value. This influence it is not observed for temperatures below $k_BT = 0.03$, then for higher temperatures the dynamics is more similar to a free dissipation dynamics where the uncertainty product always increases with time.



(a) Friction coefficient (b) Temperature

Figure 7: In the left panel, the uncertainty product used $k_BT = 0$ and the different friction coefficients are $\alpha_R = 0.1$, blue curve, $\alpha_R = 0.12$, red curve,$\alpha_R = 0.15$, green curve,$\alpha_R = 0.18$, orange curve. In the right panel, there is $\alpha_R = 0.2$ and the different temperatures are $k_BT = 0$, blue curve, $k_BT = 0.01$, red curve, $k_BT = 0.03$, green curve, $k_BT = 0.05$, orange curve, $k_BT = 0.1$, black curve.

4.2 Stretched Gaussian wave packet

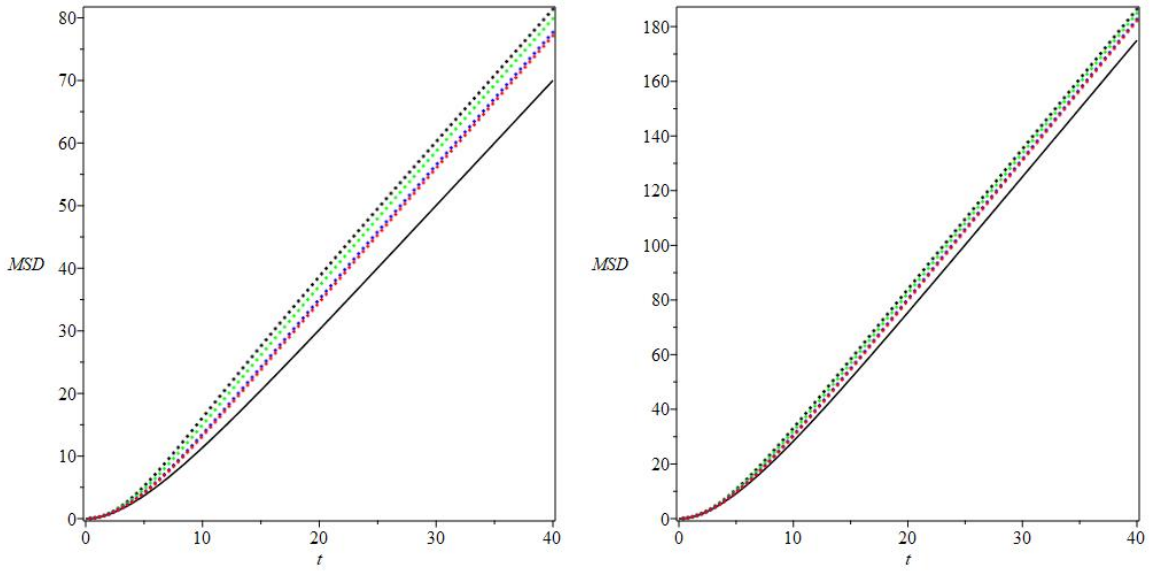
The stretching factor changes the width amplitude and it makes a different evolution for the system while the Langevin equation remains unchanged.

For the mean squared displacement and the diffusion coefficient, the stretching factor has values between 0 and 1, while the temperature and friction coefficient have the same values considered for the Gaussian wave packet. In this case, the time evolution for different temperatures is divided into two different plots to have a better evaluation from the contribution of the stretching factor.

The mean squared displacement is given in Fig.8. The effect of the stretching factor reduces the difference between the classical and quantum regime. The stretching factor can be considered when the width value is not clearly defined and gives a possible spectrum of values.

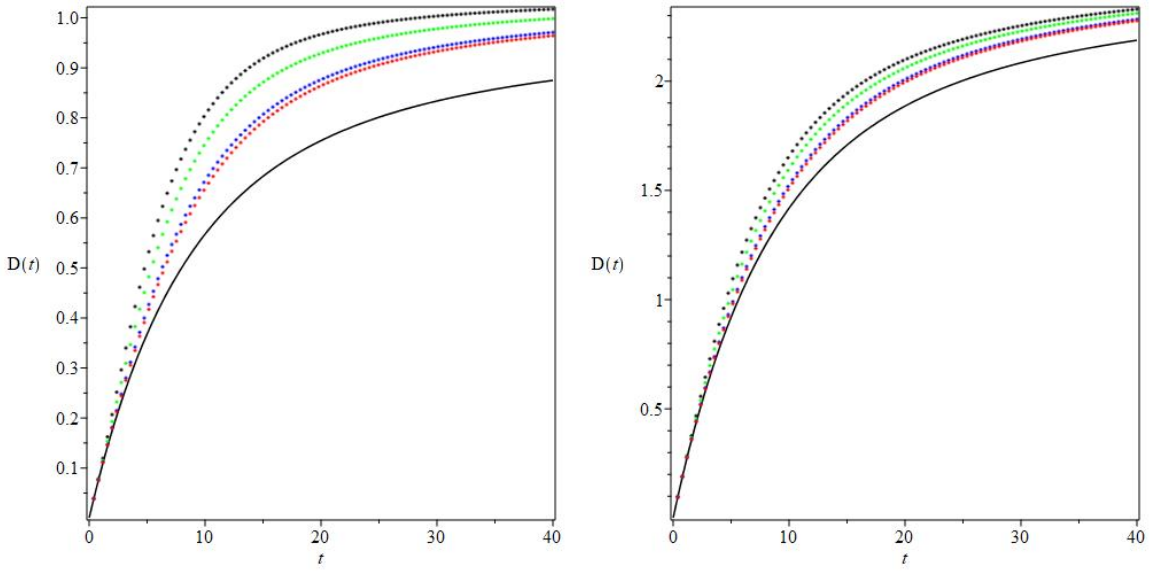
The diffusion coefficient is in Fig.9. The stretching factor reduces the difference between classical and quantum regime as in the mean squared displacement. The asymptotic value is still greater in the quantum regime than in the classical regime.

The uncertainty product uses the stretching factor $\eta = 1$ to compare with the



(a) $k_BT = 0.2$ (b) $k_BT = 0.5$

Figure 8: The mean squared displacement with $\alpha_R = 0.2$ for the quantum values are the dotted curves and for the classical values are the solid curves. The different stretching factor are $\eta = 0$ in black, $\eta = 0.5$ in green, $\eta = 0.9$ in blue and $\eta = 1$ in red. The temperature is indicated below the image.

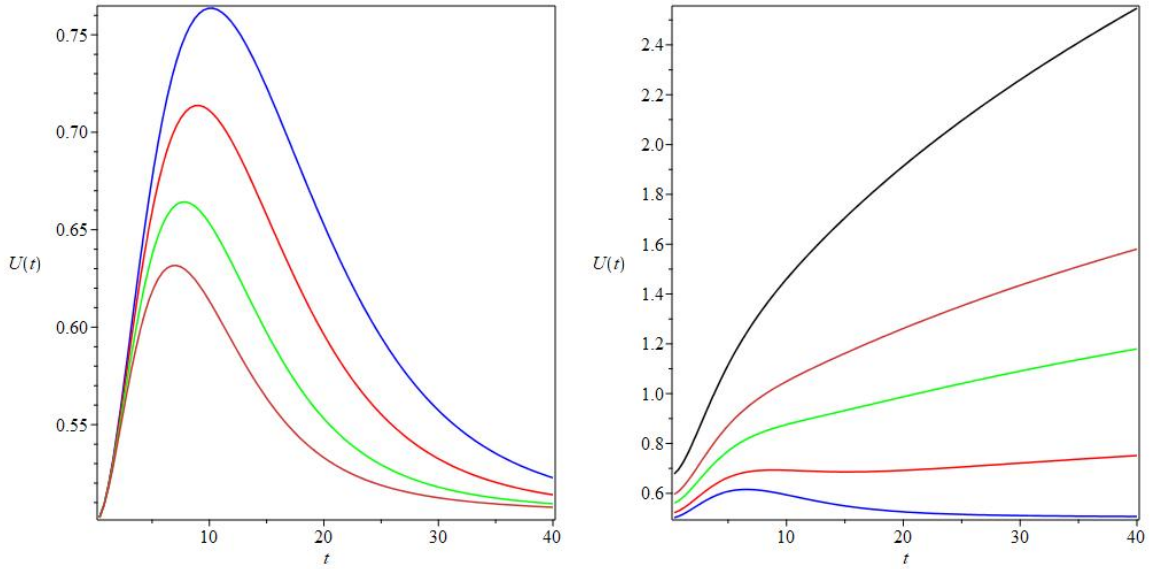


(a) $k_BT = 0.2$ (b) $k_BT = 0.5$

Figure 9: The diffusion coefficient with $\alpha_R = 0.2$ for the quantum values are the dotted curves and for the classical values are the solid curves. The different stretching factor are $\eta = 0$ in black, $\eta = 0.5$ in green, $\eta = 0.9$ in blue and $\eta = 1$ in red. The temperature is indicated below the image.

Gaussian wave packet. For this, there is a study for the friction coefficient and one for the temperature in Fig.10. The analysis of the form for the time evolution is the same as the Gaussian wave packet, but the amplitude of the maximum of the different friction

coefficient is reduced about half respect the initial value. The different temperatures are more separated at the initial time between them respect to the Gaussian wave packet.



(a) Friction coefficient (b) Temperature

Figure 10: The uncertainty product for stretching factor $\eta = 1$. In the left panel, it used $k_BT = 0$ and the different friction coefficients are $\alpha_R = 0.1$, blue curve, $\alpha_R = 0.12$, red curve,$\alpha_R = 0.15$, green curve,$\alpha_R = 0.18$, orange curve. In the right panel, there is $\alpha_R = 0.2$ and the different temperatures are $k_BT = 0$, blue curve, $k_BT = 0.01$, red curve, $k_BT = 0.03$, green curve, $k_BT = 0.05$, orange curve, $k_BT = 0.1$, black curve.

5 Conclusions

This work proves the non linear Schrödinger equation for open quantum systems from the Caldeira- Leggett Hamiltonian. The non linear becomes a system with stochastic force modelling the behaviour of the environment and a friction term associated with the contact between the system and the reservoir. After that, this equation is applied to describe the Brownian-Bohmian motion.

The theoretical development has been satisfying because the Kostin procedure with its subsequent generalization and the scale relativity method obtain the same Schrödinger- Langevin equation from the Langevin equation of motion. The Kostin procedure is a heuristic method which is very intuitive with the quantum mechanics operators. The generalization uses a classical description to obtain a similar development, but it becomes incomplete because it does not give the form of $W(t)$. The scale

relativity method is an alternative theory with a high potential because it relates the classical mechanics with the quantum mechanics by a fractal description of the space-time.

The application of the work to the Brownian motion has also been good. The wave packet center for the Gaussian and stretched Gaussian wave packets has the same evolution as the classical equation derived from the Caldeira-Leggett Hamiltonian. Then, the general center of the wave packet distribution can be considered classical and the quantum regime is shown in the width, which contains the different information between the Gaussian and stretched Gaussian wave packet. It implies the quantum behaviour of the particle depends on its width.

The Bohmian stochastic trajectories are an important result from the Brownian-Bohmian motion and they come from the classical stochastic Langevin equation of the wave packet with the damped Pinney equation related to the width evolution. The importance of the stochastic force is seen in the randomness of the trajectories with a higher values of the temperature. This randomness of the trajectories displays the importance of the averaged quantities because it is impossible to take good measures for only one stochastic trajectory.

Regarding the results for the wave packets, the studied characteristics of Brownian motion have been correctly shown because the diffusion coefficient and the mean squared displacement are higher with the temperature. The diffusion coefficient has an asymptotic value for higher times as the Einstein relation indicates. The Heisenberg minimum uncertainty product is corroborated and the Gaussian distribution is proved as the minimum uncertainty wave packet since the asymptotic values without random force is the minimum value.

The description of the stretched Gaussian wave packet has not been done before in the literature. The equations of motion obtained are a Langevin equation for the center position, Eq.(147), and a Ermakov generalized or damped Pinney equation for the width, Eq.(148). The damped Pinney equation is a new generalization and it has not been defined in previous research. With these equations, the numerical calculations for the Brownian-Bohmian motion has been performed where the coefficient diffusion has a dependence on the stretching factor for the quantum regime while the classical one is the same as the Gaussian wave packet, Eq.(180). The coefficient diffusion for

the quantum regime and the uncertainty product study for this type of wave packet, Eq.(198), is original of this work.

The results for the stretched Gaussian wave packet have not shown significance differences in behaviour over time. The diffusion coefficient approaches the evolution of the classical regime with the higher values of stretching factor, so the stretching factor tends to infinity can be considered as a possible classical approximation.

The stretched Gaussian wave packet is a generalization of the Gaussian wave packet where the mathematical issues have the same complexity. It can be used as Gaussian system with undetermined width where the stretching factor can model this indeterminacy.

The ways to continue this work is the representation of other applications of the theoretical work development in this paper such as Zeno effect or the application of a electromagnetic field. It can be considered the study of the stretching factor tends to infinite as classical limit, where the space probability to find the particle is expanded as a more delocalised distribution. The stretched Gaussian wave packet can be applied to other types of motion beyond the Brownian motion.

6 Appendix

6.1 Expected position and probability current

The expected position for an operator is

$$\langle x \rangle = \int \psi^* x \psi dx \qquad , \tag{200}$$

with the time derivative associated

$$\frac{d}{dt}\langle x \rangle = \int \left[\frac{d\psi^*}{dt} x\psi + \psi^* x \frac{d\psi}{dt} + \psi^* \frac{dx}{dt}\psi \right] dx \qquad . \tag{201}$$

For the wave function and the complex conjugate, the time derivative can be determined by the Schrödinger equation

$$\frac{d\psi}{dt} = \frac{-i}{\hbar} H\psi \tag{202}$$

and the time derivative with the Schrödinger equation is

$$\frac{d}{dt}\langle x\rangle = \int \left[\frac{i}{\hbar}H\psi^* x\psi + \psi^* x\frac{(-i)}{\hbar}H\psi + \psi^*\frac{dx}{dt}\psi\right]dx \qquad . \tag{203}$$

The Hamiltonian considered in this work is

$$H = \frac{1}{2m}(-i\hbar\frac{d}{dx})^2 + V \qquad , \tag{204}$$

where the first term is the kinetic part and the other is a potential considered real. With this Hamiltonian, the expected position value can be reduced as

$$\frac{d}{dt}\langle x\rangle = \int \frac{i}{2m\hbar}\left[(i\hbar\frac{d}{dx})^2\psi^* x\psi - \psi^* x(-i\hbar\frac{d}{dx})^2\psi\right]dx + \int \psi^*\frac{dx}{dt}\psi dx \qquad . \tag{205}$$

It reads

$$\frac{d}{dt}\langle x\rangle = \int \frac{-i\hbar}{2m}\left[\frac{d}{dx}\psi^*\psi - \psi^*\frac{d}{dx}\psi\right]dx + \int \psi^*\frac{dx}{dt}\psi dx \qquad . \tag{206}$$

At this point, the definition of the probability current, Eq.(82), is introduced

$$\frac{d}{dt}\langle x\rangle = \int J dx + \langle\frac{dx}{dt}\rangle \qquad , \tag{207}$$

and with the final consideration that the average value of the velocity is centered on the origin

$$\frac{d}{dt}\langle x\rangle = \int J dx \qquad . \tag{208}$$

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