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NUMERICAL STUDIES OF THE STOCHASTIC, DISCRETE, NONLINEAR SCHRÖDINGER EQUATION

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Abstract

We analyse properties of non-linear, stochastic dimer (a system consisting of two lattice sites with stochastic energies) using the discrete, nonlinear, Schrödinger equation. The aim is to obtain a solution of such systems, mainly through numerical studies. Analytical studies has been taken only in the limiting case where the standard deviation is small enough and the correlation time quite large.

With the advent of low stochastic effect, it seems that, with nonlinearity increasing, the mean value of the probability difference (for the particle to be at site 1 or 2) , is descending quickly, to an "equilibrium" value. After the advent of strong stochastic processes, the main conclusion is just the following. The mean value of the probability difference , under stochastic processes and after an interval time , tends to zero. This situation takes place for any value of nonlinearity. The "force" of nonlinearity tries to keep the system in an "equilibrium" value. However, under stochastic processes constraint, the probability difference tends again to zero.

With a large stochastic effect and without nonlinearity, the system behaves like sub-diffusion. The diffusion comes as a limiting case when the correlation time get large value. In contrast, if we put together, a low stochastic effect with nonlinearity, we obtain a hypertransport phenomenon. Again, the ballistic transport can be possible when nonlinearity approaches marginally the unit.

Contents

1 Acknowledgments

First, I would like to thank my supervisor, Giorgos Tsironis, for introducing me into the physics of non-linear phenomena and giving me the opportunity to work on such a fascinating subject as the analysis of the behavior of the Discrete Non-Linear Schrödinger (DNLS) equation on dimer . I am grateful for his guidance, encouragement and trust during this work. I feel very grateful to my coleagues, the people I worked with during my stay in Professor Tsironis' group. Particularly, Nikos Lazarides, Basilis Paltoglou, Marios Mattheakis and Nikos Tsatrafilis were always there to listen and help me with my Master Thesis giving me advices. During my Master Programm, I had the luck to be hosted in a very nice room in the 2nd floor of the Physics Depatment, were some very intresting people were hosted too. Bagelis Karamanos, Xara Troullinou and Dimitris Markelos were the best group of students that one needs to have close to him to be productive and extreamlly contented while working.

I also want to thank my spiritual friend Gianis Iatrakis for on our endless scientific discussions and my friends Stergios and Aleksandra for them psychological support.

Last but not least, I would like to thank my family: my parents, Karafil , Mirieta and my sister, Salida, for being always next to me, helping me and supporting me, even when I turned to be a great trouble, and my Aggeliki for cheering me up when I had bud time.

2 INTRODUCTION

The discrete nonlinear Schrödinger equation (DNLS) describes properties of chemical, condensed matter as well as optical systems where self-trapping mechanisms are present. These mechanisms arise from strong interaction with the environment or genuine nonlinear properties of the medium. The DNLS was introduced in order to describe the dynamics of a set of nonlinear anharmonic oscillators and understand nonlinear localization phenomena. It can also be viewed as an equation describing the motion of a quantum mechanical particle interacting strongly with vibrations.

If $c_n(t)$ denotes the probability amplitude for the particle to be at site n at time t, the DNLS reads

$$i\frac{dc_n}{dt} = \epsilon_n c_n + V(c_{n-1} + c_{n+1}) - \chi|c_n|^2 c_n \tag{2.1}$$

where ϵ_n designate the local energies at site n of an one-dimensional crystal, V is the nearest-neighbor wavefunction overlap and χ is the nonlinearity parameter that is related to the interaction of the particle with other degrees of freedom of the medium.

One of the few analytically solvable cases that provides substantial intuition on the properties of Eq.2.1 is that of a system consisting of two lattice sites with different energies. With that in our mind, we have a differential system and we obtain the following equations,

$$i\frac{dc_1}{dt} = \epsilon_1 c_1 + V c_2 - \chi|c_1|^2 c_1^* \tag{2.2}$$

$$i\frac{dc_2}{dt} = \epsilon_2 c_2 + V c_1 - \chi|c_2|^2 c_2^* \tag{2.3}$$

We first derive from Eq.2.2, Eq.2.3 the corresponding Liouville-Von Neumann equation for the density matrix elements ρ_{mn}.

$$i\dot{c_1}c_1^* = \epsilon_1|c_1|^2 + Vc_2c_1^* - \chi|c_1|^4 \tag{2.4}$$

$$i\dot{c_1}^*c_1 = -\epsilon_1|c_1|^2 - Vc_2^*c_1 + \chi|c_1|^4 \tag{2.5}$$

So we have,

$$i\dot{\rho_{11}} = -V(\rho_{12} - \rho_{21}) \tag{2.6}$$

In the same way we obtain the following equations,

$$i\dot{\rho_{22}} = V(\rho_{12} - \rho_{21}) \tag{2.7}$$

$$i\dot{\rho_{12}} = (\epsilon_1 - \epsilon_2)\rho_{12} - V(\rho_{11} - \rho_{22}) - \chi\rho_{12}(\rho_{11} - \rho_{22}) \tag{2.8}$$

$$i\dot{\rho_{21}} = -(\epsilon_1 - \epsilon_2)\rho_{21} + V(\rho_{11} - \rho_{22}) + \chi\rho_{21}(\rho_{11} - \rho_{22}) \tag{2.9}$$

If we call $\epsilon'(t) = \epsilon_1 - \epsilon_2$ then we have,

$$i\frac{d}{dt}(\rho_{11} - \rho_{22}) = -2V(\rho_{12} - \rho_{21}) \tag{2.10}$$

$$i\frac{d}{dt}(\rho_{12}-\rho_{21}) = \epsilon'(t)(\rho_{12}+\rho_{21})-2V(\rho_{11}-\rho_{22})-\chi(\rho_{11}-\rho_{22})(\rho_{12}+\rho_{21}) \tag{2.11}$$

$$i\frac{d}{dt}(\rho_{12} + \rho_{21}) = \epsilon'(t)(\rho_{12} - \rho_{21}) - \chi(\rho_{11} - \rho_{22})(\rho_{12} - \rho_{21}) \tag{2.12}$$

Now we set $P = \rho_{11} - \rho_{22}$, $Q = \rho_{12} - \rho_{21}$, $R = \rho_{12} + \rho_{21}$. So, we obtain,

$$\dot{P} = -2VQ \tag{2.13}$$

$$\dot{Q} = R - 2VP - \chi PR \tag{2.14}$$

$$\dot{R} = Q + \chi PQ \tag{2.15}$$

and introduce the last transform $p = P, q = iQ, r = R, \tau = 2Vt, \epsilon = \frac{\epsilon'}{2V}, g = \frac{\chi}{2V}$ we finally obtain,

$$\dot{p} = q \tag{2.16}$$

$$\dot{q} = \varepsilon r - q - gpr \tag{2.17}$$

$$\dot{r} = \varepsilon q + gpq \tag{2.18}$$

The main concern from now on, in this thesis, will be the solution of the above system.

3 ANALYTICAL STUDIES

3.1 Stochastic processes

It is well known that a particle moving in a spatially disordered time-independent potential can exhibit Anderson localization and that this is the generic situation in one or two dimensions. If the potential fluctuates in time as well as in space, the arguments will lead to Anderson localization break down[1]. When Anderson localization is destroyed, it will be replaced by diffusive transport. So, if we want to see diffusive transport in a lattice we must have a disorder time-depended potential.

To our problem the local energies, at both sites, are taken to be stochastic or random in time. This means that the energy ϵ satisfy a stochastic differential equation

$$\dot{\epsilon(\tau)} = \frac{\epsilon(\tau) - \Gamma(\tau)}{t_c} \tag{3.1}$$

where $\Gamma(\tau)$ is a random function (Langevin force) with the following properties.

a. Its average over the ensemble should be zero:

$$< \Gamma(\tau) >= 0 \tag{3.2}$$

[1]Applications in optics:
In experiments examining Anderson localization of light, the potential was realized by a superposition of plane waves. In those experiments light propagates paraxially in a disordered potential: the signature of localization is that the width of the propagating beam of light from a coherent and a monochromatic source remains bounded as it propagate. The disordered potential is produced by utilizing the photosensitivity of the medium. A powerful polarized writing beam induces a change in the refractive index of the medium. The polarization of this beam is selected in such a manner that the beam does not experience the change in the refractive index that is induce. The localization experiments are carried out with another beam with a different polarization, such that it experiences the written change in the refractive index.

b. If we multiply two Langevin forces at different times we assume that the average value is:

$$< \Gamma(\tau)\Gamma(\tau') >= q\delta(\tau - \tau') \tag{3.3}$$

where $q = const^2$.

c. We assume that the random variables $\Gamma(\tau)$, for each time point, are distributed according to the Gaussian distribution function with zero mean and a particular standard deviation.

The symbol t_c is the correlation time. The smaller the times the closer will be the values of random numbers and vice versa.

3.2 The linear case (with large t_c and small σ)

Suppose that we have two random values $\epsilon(\tau_1)$ and $\epsilon(\tau_2)$. Since $\epsilon(\tau)$ depends linearly on the random variables $\Gamma(\tau)$, it must follow a Gaussian distribution function with zero mean and a particular standard deviation. If the correlation time is large enough then, through the equation

$$< \epsilon(\tau_1)\epsilon(\tau_2) >= \frac{D}{2t_c} e^{-1/t_c|\tau_1 - \tau_2|} \tag{3.4}$$

it becomes clear that the correlation for the random values of $\epsilon(\tau_1)$ and $\epsilon(\tau_2)$ will be very small (see Appendix A.3). This means that, if we take a value from a "box" with random numbers, e.g $\epsilon(\tau_1)$, the second choice, from the same "box", will have a value close to the first one, e.g $\epsilon(\tau_1) \simeq \epsilon(\tau_2)$. Finally, with the above condition where the correlation time is quite large, we can assume that $\epsilon(t)$ is constant.

[2] In our numerical study $q = \frac{\sigma^2}{2h}$ where σ will be the standard deviation of energy-random variables distribution and h the step of Heun routine. This is a routine which solves a system of first order (see Appendix A.2).

If we set $\epsilon_(\tau) = constant$, the solution for the differential system (2.16,2.17,2.18, for the linear case where $g = 0$, is quite simple. For the initial values $p(0) = 1, q(0) = 0, r(0) = 0)$ we obtain,

$$\dot{r(\tau)} = -\epsilon \dot{p(\tau)} \Rightarrow \int_0^\tau \frac{dr}{d\tau}\tau = -\epsilon \int_0^\tau \frac{dp}{d\tau} d\tau \Rightarrow r(\tau) = -\epsilon(p(\tau) - 1) \quad (3.5)$$

then,

$$\ddot{p} + (1 + \epsilon^2) = \epsilon^2 \quad (3.6)$$

with finally solution,

$$p(\tau) = \frac{1}{1 + \epsilon^2} \cos\tau(\sqrt{1 + \epsilon^2}) + \frac{\epsilon^2}{1 + \epsilon^2} \quad (3.7)$$

We can observe that for $\epsilon = 0$ the solution will have the simple form

$$p(\tau) = \cos(\tau) \quad (3.8)$$

What interest us is the mean value of $p(\tau)$ (ϵ are stochastic variables) and is defined as:

$$< p(\tau) >= \int_{-\infty}^{\infty} p(\tau) P(\epsilon) d\epsilon \quad (3.9)$$

where $P(\epsilon)$ is the distribution of energy random values. From the above analysis $P(\epsilon)$ should be in the form of a Gaussian distribution:

$$P(\epsilon) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-\epsilon^2}{2\sigma^2}} \quad (3.10)$$

To calculate the integral of Eq. 3.9 we assume that $\frac{1}{\sigma^2}$ is large (the standard deviation σ quite small). We can apply Laplace's method of integration [3]

[3]Consider an integral of form:

with relative error $O(\lambda^{-1})$ where $\lambda = \frac{1}{\sigma^2}$. The minimum of the function $\frac{-\epsilon^2}{2}$ is to $\epsilon = 0$. After some calculations we obtain:

$$< p(\tau) > \simeq \cos(\tau) \tag{3.17}$$

with relative error $O(\sigma^2)$. This approach reveals that the mean value of the probability difference $< P(\tau) >$, for standard deviation being quite small, has the same behaviour with $P(\tau)$, when the energy of the last (remember, the difference of energies at sites 1 and 2) is zero Eq. 3.8.

$$I = \int_a^b e^{-\lambda g(y)} h(y) dy \tag{3.11}$$

here λ is large, $g(y)$ is a smooth function which has a local minimum at $y*$ in the interior of the interval (a,b) and $h(y)$ is smooth

When λ is large, the contribution to this integral is essentially entirely originating from a neighbourhood around $y*$. We formalize this by Taylor expansion of the function g around $y*$.

$$g(y) = g(y^*) + g'(y^*)(y - y^*) + g"(y^*)(y - y^*)^2/2 + ... \tag{3.12}$$

Since y^* is a local minimum, we have $g'(y^*) = 0$, $g"(y^*) > 0$ and thus

$$g(y) - g(y^*) = g"(y^*)(y - y^*)^2/2 + ... \tag{3.13}$$

If we farther approximate $h(y)$ linearly around $y*$ we get:

$$\int_{-\infty}^{\infty} e^{-\lambda g(y)} h(y) dy \simeq e^{-\lambda g(y^*)} h(y^*) \int_{-\infty}^{\infty} e^{-\lambda g"(y^*)(y-y^*)^2/2} dy \tag{3.14}$$

$$+ e^{-\lambda g(y^*)} h'(y^*) \int_{-\infty}^{\infty} (y - y^*) e^{-\lambda g"(y^*)(y-y^*)^2/2} dy \tag{3.15}$$

The critical point is that the second term go to zero because it have a Gaussian integrate form. In our cases the special form of Gaussian distribution lead, any second order approximation of $h(y)$, to zero.

The final answer of the problem is

$$I \simeq e^{-\lambda g(y^*)} h(y^*) \sqrt{\frac{2\pi}{\lambda g"(y^*)}} \tag{3.16}$$

$$< p(\tau) > \simeq P(\tau)|_{\epsilon=0} \tag{3.18}$$

3.3 The nonlinear case (with large t_c and small σ)

As in the linear case, so also for the nonlinear case we assume that, for the differential system (Eq. 2.16,2.17,2.18), $\epsilon(\tau) = constant$. In the same way, for this case, the correlation time must be large enough. The only difference is that now we have nonlinearity $g \neq 0$. With the same initial conditions as before, $p(0) = 1, q(0) = 0, r(0) = 0$), if we put 2.17 in 2.16, we obtain:

$$\ddot{p} = \epsilon r - p - gpr \tag{3.19}$$

From Eq. 2.18, by integration with respect to time and for $r(0) = 0, p(0) = 1$ we have:

$$r = -\epsilon p + \epsilon + \frac{g}{2}p^2 - \frac{g}{2} \tag{3.20}$$

Putting the above equation in Eq. 3.19 we obtain:

$$\ddot{p} = a_1 p^3 + a_2 p^2 + a_3 p + a_4 \tag{3.21}$$

where $a_1 = -\frac{g^2}{2}, a_2 = \frac{3\epsilon g}{2}, a_3 = \frac{g^2}{2} - g\epsilon - \epsilon^2 - 1, a_4 = \epsilon^2 - \frac{g\epsilon}{2}$.

Because $\frac{d}{dt}(\dot{p})^2 = 2\dot{p}\ddot{p}$ by integration again, with respect to time, and after some calculations we obtain:

$$\dot{p}^2 = (1 - p)(a_0 p^3 + a_1 p^2 + a_2 p + a_3) \tag{3.22}$$

where now:

$$a_0 = \frac{g^2}{4} = (\zeta)^2 \tag{3.23}$$

$$a_1 = \frac{g^2}{4} - \epsilon g = (\zeta)(\zeta + 2\epsilon) \tag{3.24}$$

$$a_2 = -\frac{g^2}{4} + \epsilon^2 + 1 = \epsilon^2 - (\zeta)^2 + 1 \tag{3.25}$$

$$a_3 = -\frac{g^2}{4} + g\epsilon - \epsilon^2 + 1 = 1 - (\epsilon + \zeta)^2 \tag{3.26}$$

with $\zeta = \frac{g}{2}$ and a well-known root of the polynomial $P_0 = 1$. Using another simple transformation we obtain:

$$\dot{p}^2 = a'_0 p^4 + 4a'_1 p^3 + 6a'_2 p^2 + 4a'_3 p + a'_4 \tag{3.27}$$

where

$$a'_0 = -a_0 \tag{3.28}$$

$$4a'_1 = (a_0 - a_1) \tag{3.29}$$

$$6a'_2 = (a_1 - a_2) \tag{3.30}$$

$$4a'_0 = (a_2 - a_3) \tag{3.31}$$

$$a'_4 = a_3 \tag{3.32}$$

where we have again as a root of the polynomial $P_0 = 1$. The solution of the above differential is[4]:

[4] If we want to evaluate t integrals in the form:

$$\int \frac{dx}{\sqrt{f(x)}} \tag{3.33}$$

for the polynomial $f(x) = a_0 x^4 + 4a_1 x^3 + 6a_2 x^2 + 4a_3 x + a_4$ we form the invariants:

$$\ell_2 = a_0 a_4 - 4a_1 a_3 + 3a_2^2 \tag{3.34}$$

$$\ell_3 = a_0 a_2 a_4 + 2a_1 a_2 a_3 - a_2^3 - 3a_0 a_3^2 - a_1^2 a_4 \tag{3.35}$$

$$p(\tau) = P_0 + \frac{1}{4}\{\frac{P'(P_0)}{W(\tau;\ell_2;\ell_3) - \frac{1}{24}P''(P_0)}\} \tag{3.38}$$

where

$$\ell_2 = a'_0a'_4 - 4a'_1a'_3 + 3(a'_2)^2 \tag{3.39}$$

$$\ell_3 = a'_0a'_2a'_4 + 2a'_1a'_2a'_3 - (a'_2)^3 - a'_0(a_3)')^2 - a'_4(a'_1)^2 \tag{3.40}$$

and $W(\tau;\ell_2;\ell_3)$ is the Weierstrass elliptic function.

As in the linear case, what interest us is the mean value of $p(\tau)$. It have the same definition with equation 3.9. Again, to calculate the integration of 3.9 (with $p(\tau)$ at this time the Weierstrass elliptic function) we assume that $\frac{1}{\sigma^2}$ is large (the standard deviation σ quite small). Using Laplace's method and knowing that the minimum of $\frac{-\epsilon^2}{2}$ happen when $\epsilon = 0$, we demand that:

$$< p(\tau) >= p(\tau))|_{\epsilon=0} \tag{3.41}$$

With that demand and after some calculations we obtain:

$$< p(\tau) >= 1 - \frac{1}{4}\{\frac{4\zeta^2 + 2}{W(\tau;\ell_2;\ell_3) + \frac{1}{12}(\zeta^2 + 2)}\} \tag{3.42}$$

where

$$\ell_2 = \frac{4}{3}(\zeta^4 - \zeta^2) + \frac{1}{12} \tag{3.43}$$

Let:

$$z = \int_{x_0}^{x} \frac{dt}{\sqrt{f(t)}} \tag{3.36}$$

where x_0 is a root or the equation $f(x) = 0$. Indicating the Weierstrass elliptic function as $W(z;\ell_2;\ell_3)$, the solution of integral, for $x = x(z)$ is:

$$x = x_0 + \frac{1}{4}\{\frac{f'(x_0)}{W(z;\ell_2;\ell_3) - \frac{1}{24}f''(x_0)}\} \tag{3.37}$$

$$\ell_3 = \frac{\zeta^2 + 36(2\zeta^6 - 3\zeta^4) - (8\zeta^6 - 12\zeta^4 + 6\zeta^2 - 1)}{216} \tag{3.44}$$

The dynamical properties of a system consisting of two lattice sites with equal energies have been studied extensively. This means that in our case $\epsilon = \frac{\varepsilon_1 - \varepsilon_2}{2} = 0$. The solutions presented in these studies are related to the value of ζ. For $0 \leq \zeta < 1$ the probability difference displays oscillations about the value 0 , and is given by:

$$p(\tau) = cn(\tau|k = \zeta) \tag{3.45}$$

whereas, for $\zeta > 1$, the probability difference oscillates only on one site of 0 and is explicitly given by:

$$p(\tau) = dn(\tau\zeta|k = \zeta) \tag{3.46}$$

where k is the respective elliptic parameter of the Jacobian elliptic function cn and dn . In numerical studies we will show that Eq. 3.42 has the same behaviour with the above Jacobian function. Again, as in the linear case, the mean value of probability difference $< P(\tau) >$, for standard deviation quite small, has the same behaviour with $P(\tau)$ when the difference of energies at sites 1 and 2 is zero.

4 NUMERICAL STUDIES

4.1 Numerical Procedure

As we observed, analytical solution of the system of differential equations, (2.16, 2.17, 2.18), we can have only in special cases. In the above analytical studies we made two significant approximations. The first one was the time independence of energy differences and the second one was the calculation of distribution with the Laplace approximation.In both cases, we assumed large correlation time and standard deviation quite small. To go further in the solution understanding, we should take into consideration all cases (time depended energy and the entire range of correlation time values as well the standard deviation values). To achieve this we proceed via numerical studies.

Initially, we write a routine which provides us with random numbers. With another routine we control if the random numbers satisfy a Gaussian distribution with a particular standard deviation. Then we solve the differential equation 3.1 where τ (the correlation time) is a parameter and $\Gamma(t)$ are the above random numbers. For each random variable ϵ (which describes the energy differences) we solve the system of differential equations 2.16 2.17 2.18, with a particular non-linear constant. In the end, we calculate the time average of $< p(\tau) >$ since the whole problem is stochastic. In this way, all the parameters of the problem are τ (the correlation time), σ (standard deviation of distribution) and g (non-linearity). Only these (parameters) will be studied, separating the problem, again, in the linear and non-linear case.

4.2 The linear case

Initially, the numerical results of the solution of our linear system should satisfy those of analytical. For this reason, with correlation time being large enough and for small enough standard deviation, we should have the same behaviour with Equation 3.17.This becomes clear in the following graphs

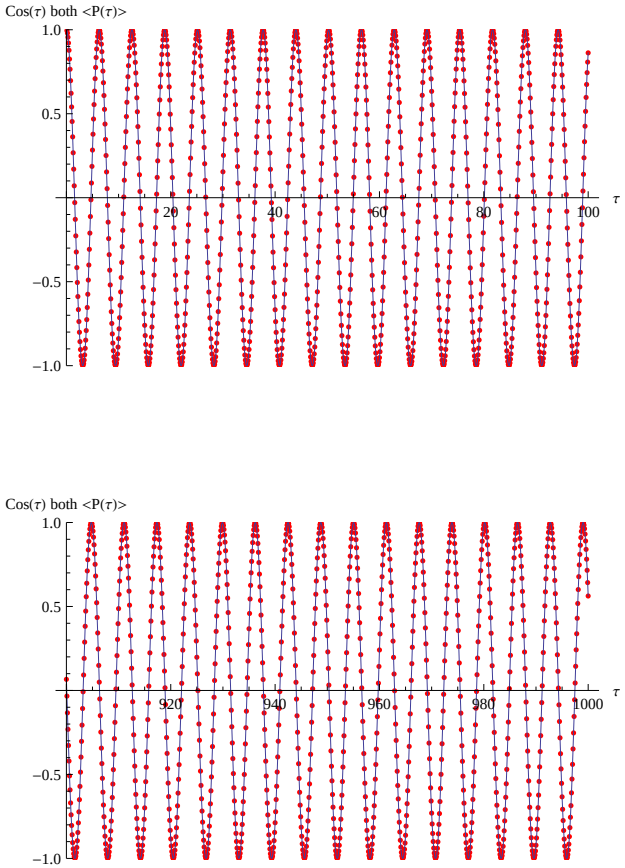


Figure 1: The numerical solution of stochastic, differential equation (2.7) with correlation time $t_c = 10$ and standard deviation $\sigma = 0.01$,(dotted line). The full line corresponds to analytical behaviour of $\cos(\tau)$ function. The second one illustrate the identical system behaviour for long time.

where the verification of Equation 3.17 is obvious.

Due to the lack of the nonlinear term, the next step is to examine the behaviour of $< P(\tau) >$ through the entire range of correlation times, as well as the standard deviation values. For a better understanding, we examine the system keeping a variable constant(t_c or σ) and changing the second (σ or t_c).

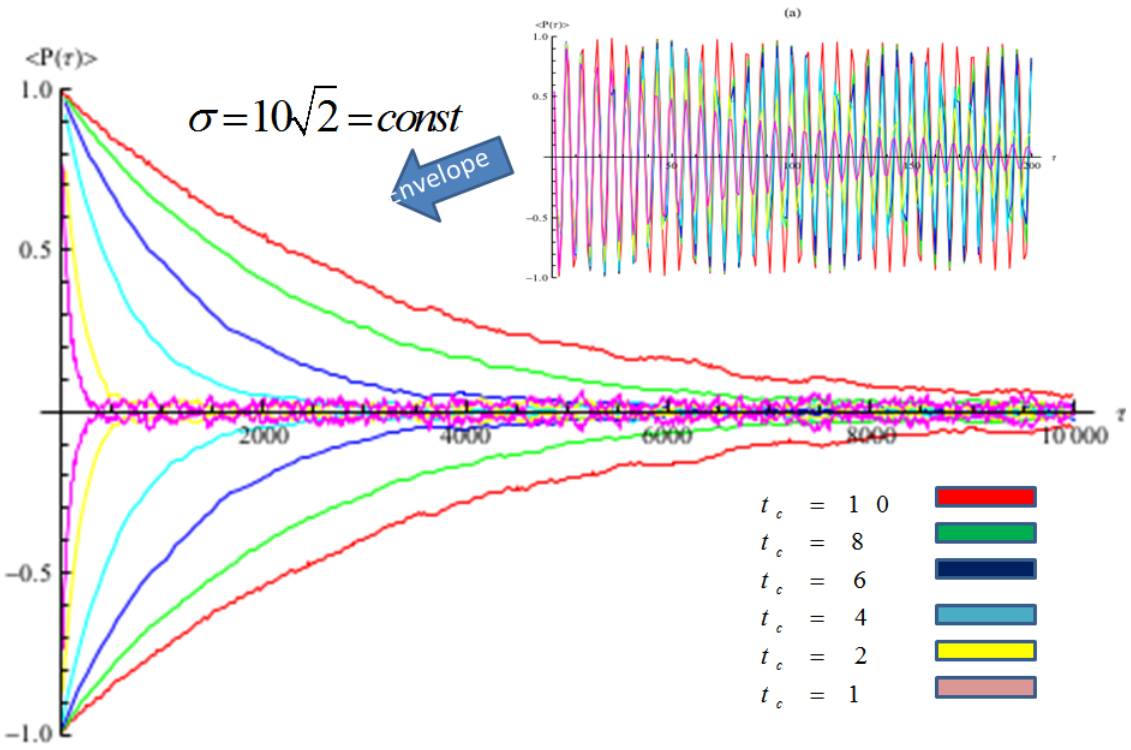


Figure 2: The probability difference as function of time. The standard deviation $\sigma = 10\sqrt{2}$ is constant. What is changing is the correlation time. Here, $t_c = 10, 8, 6, 4, 2, 1$, starting from red to lilac color where (a) corresponds to a short time interval and (b) is the envelope of $< P(\tau) >$, for a long time interval. The decrease of t_c causes a more rapid drop of $< P(\tau) >$ to zero.

In evolution of $< P(\tau) >$ as function of σ, with a constant correlation time, it is obvious(see Figure.3) that this quantity, beyond the cosine behaviour, declines versus time more sharply as the value of the standard deviation becomes higher. Similarly, keeping the standard deviation constant, the evolution of $< P(\tau) >$, as function of t_c and beyond the cosine behaviour, declines through the propagation of time. More over, the less the value of the correlation time, the sharper the declination is. (Figure.2).

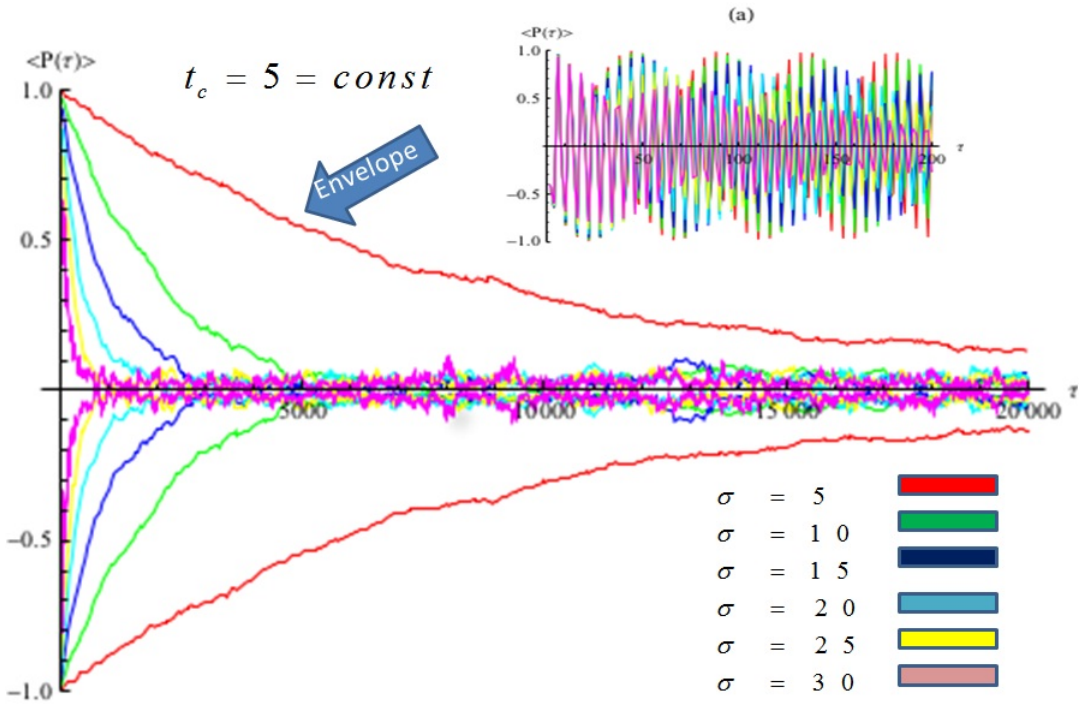


Figure 3: The probability differences as function of time. The correlation time $t_c = 5$ is constant. What changes is the standard deviation. Here, $\sigma = 5, 10, 15, 20, 25, 30$, starting from red to lilac color where (a) corresponds to a short time interval and (b) is the envelope of $< P(\tau) >$, for a long time interval. The increase of σ causes a more rapid drop of $< P(\tau) >$ to zero.

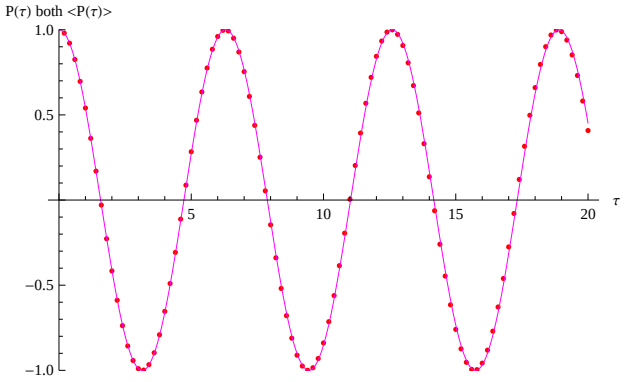
Clearly, the function of the probability differences, through an oscillatory motion and after an interval time, tends to zero. The only defined by the correlation time and the standard deviation is the time frame of such tendency.

4.3 The nonlinear case

Initially, as in the linear study also in the nonlinear one, we are looking if the numerical results keep pace with the analytical one. In the same way, the identification is being tested in the case that the correlation time, t_c, is

large and the standard deviation,σ, small enough. With very low stochastic effect (see Figure 4.), the numerical studies satisfy completely the Equation 3.42.

We must emphasize here that the solutions of differential system (Eq. 2.16,2.17,2.18) for $\epsilon = 0$ have the same form, satisfying in this way the Jacobian elliptic functions as mentioned above. It becomes clear that,for a nonlinear system with nonlinearity value near one and with the concrete, above values of t_c, σ , we meet the same qualitative change of system. For $0 \leq \zeta < 1$, the mean value of probability difference displays oscillations about the value 0 whereas, for $\zeta > 1$, the probability difference oscillates only on one site of 0.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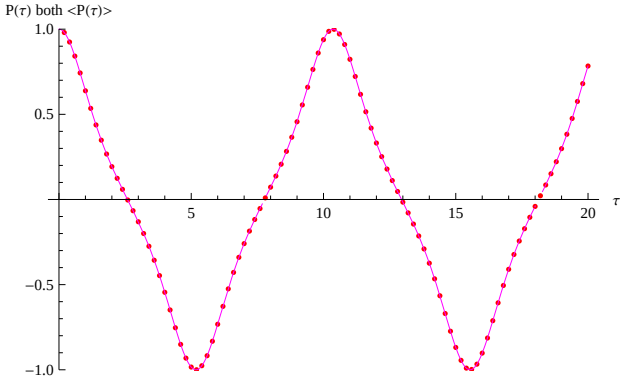
1.0
0.5
−0.5
−1.0
5
10
15
20
τ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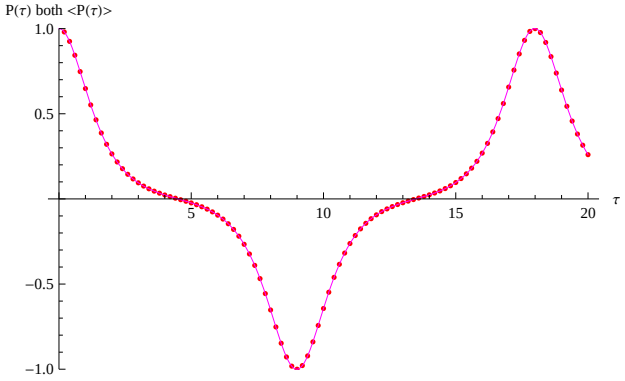
P(τ) both <P(τ)>
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−0.5
−1.0
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τ

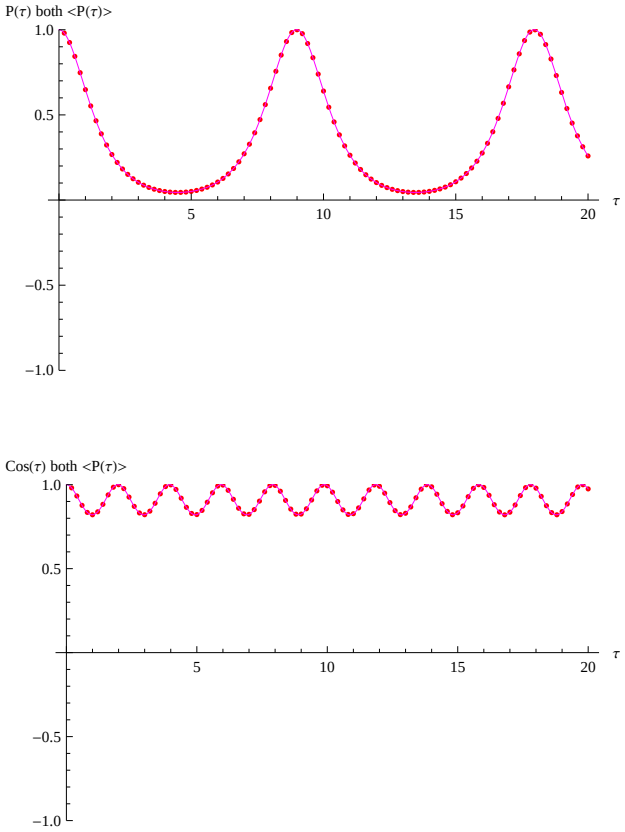

Figure 4: Starting from top to bottom, the full line shows the analytical solution of Equation3.42.Respectively, $\zeta = 0.1, 0.95, 0.999, 1.001, 1.75$ are the nonlinearity values. The dotted line is presented the numerical results, for $\tau = 100$ and $\sigma = 0.0001$. The nonlinearity values are the same.

In the above numerical calculation, in comparison with the linear case, has been obtained larger value for standard deviation σ and smaller for correlation time t_c. The reason for this is the high sensitivity of the system by the nonlinearity. This becomes clear in Figure 5.

For nonlinearity difference in the range of 0.005, and for low stochastic effect, the mean value of probability difference, $< P(\tau) >$, tends rapidly to zero. From this aspect,the primary purpose is therefore the examination of

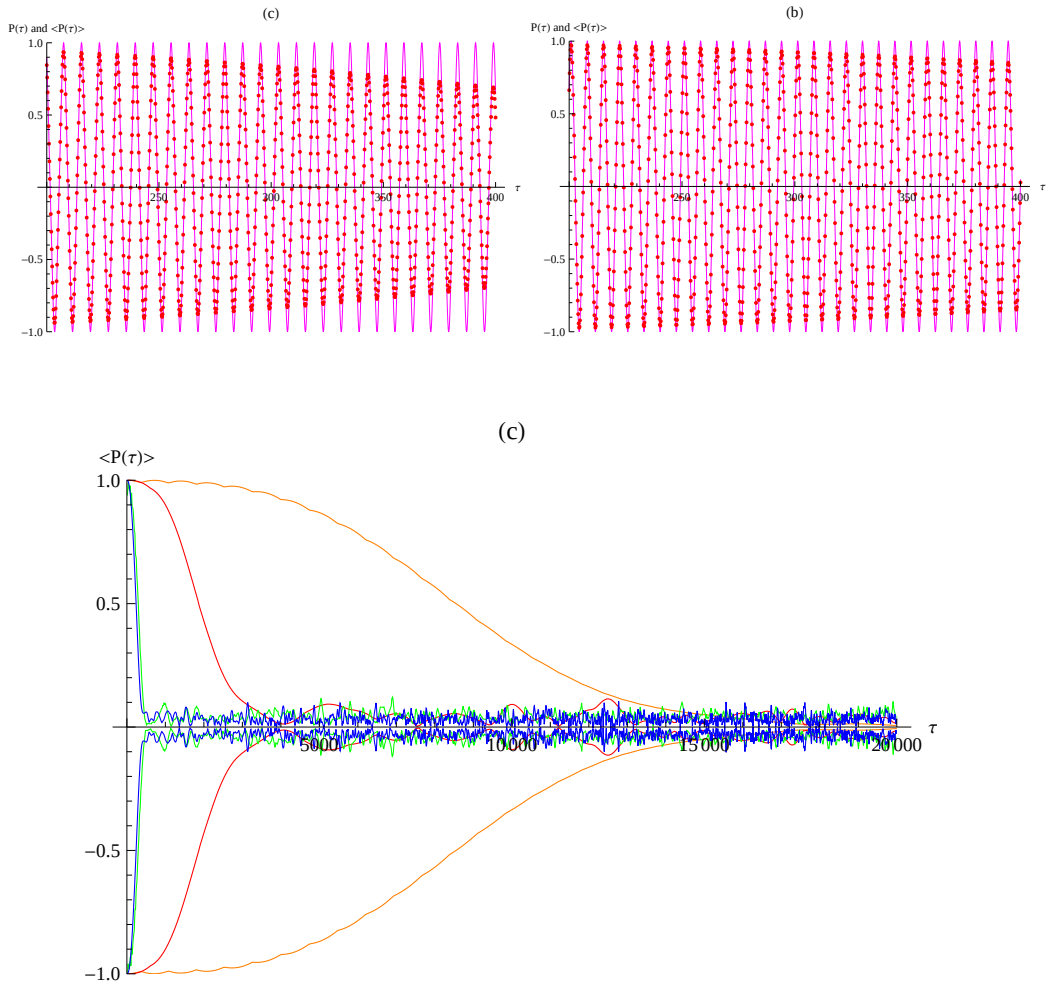

Figure 5: In the graph (c) are presented the envelope of mean values of probability differences, $< P(\tau) >$, as function of time with nonlinearity values $\zeta = 0.005, 0.05, 0.65, 0.8$ starting from orange to blue color, respectively. In (a), where $\zeta = 0.8$, and (b), where $\zeta = 0.65$, the full line shows the analytical solution of Equation3.42 while with dotted line are presented the numerical results, for a short time interval. The standard deviation value is $\sigma = 0.1$ while the correlation time is $\tau = 10$.

the system by the effect of nonlinearity.

In Figure.5 is presented the dynamical behaviour of $< P(\tau) >$. It seems

that, with nonlinearity been increased, the mean value of the probability difference, is descending quickly towards the zero. The system does not tend to zero but to a kind of equilibrium where, with $\zeta < 1$, this value, happen to be zero. As we can see in Figure 6 , this value is something like the time average of $< P(\tau) >$.

In this Figure is presented the dynamical behaviour of $< P(\tau) >$ for the nonlinearity value very close to one, from both sides. We can clearly see the system transition. For $\zeta < 1$ the evolution of $< P(\tau) >$ take place on both the positive and negative axis while, for $\zeta > 1$, is restricted only on the positive axis. In particular, the system, for $\zeta = 1.001$ and after an oscillatory motion, is descending towards a specified value. Now, it clearly seems that, this value is not zero but a "respectably" time average of $< P(\tau) >$.

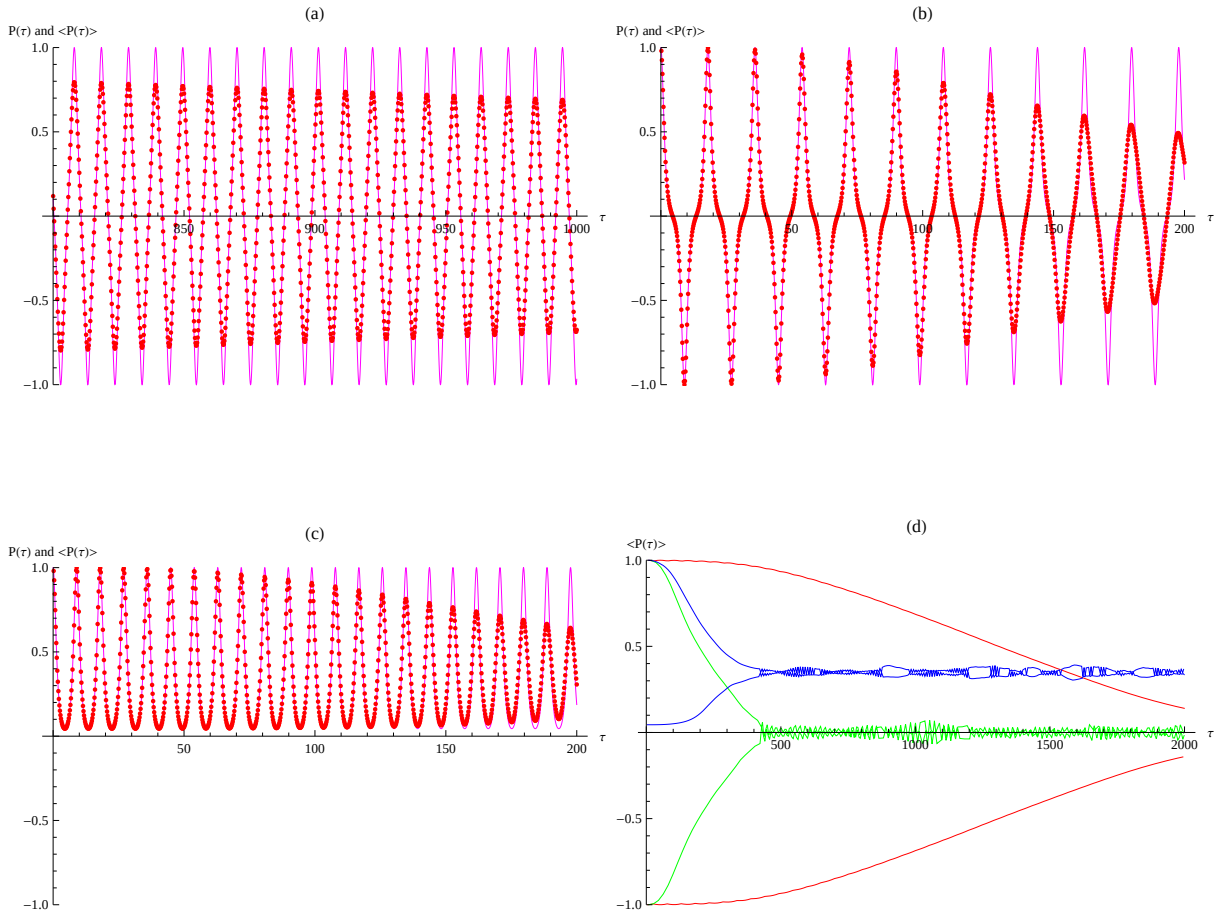

Figure 6: In the graphs, the mean value of probability difference, $< P(\tau) >$, is presented as function of time. In (a),(b),(c) where $\zeta = 0.95, 0.999, 1.001$ respectively, the full line shows the analytical solution of Equation3.42 while with dotted line are presented the numerical results, for a short time interval. In (d) is presented the envelope of $< P(\tau) >$, for a long time interval where, the (a) case is showed with red color, the (b) case with green and the (c) case with blue. The standard deviation value is $\sigma = 0.1$ while the correlation time is $\tau = 10$

Generally speaking, the nonlinearity leads the probability difference to equilibrium, destroying simultaneously, the oscillatory behaviour. The $< P(\tau) >$ obtains the equilibrium value more quickly, as the nonlinearity tends to one.

When the nonlinearity is greater than one, the evolution of the system takes place only in one site, where the mean value of the probability difference is positive. As the nonlinearity grows, the $< P(\tau) >$, after an oscillatory behaviour, tends to one Fig. 7. An oscillating behaviour is always preceded. When the nonlinearity increase, the "life time" of this oscillation has longer duration while its amplitude shrinks more and more.

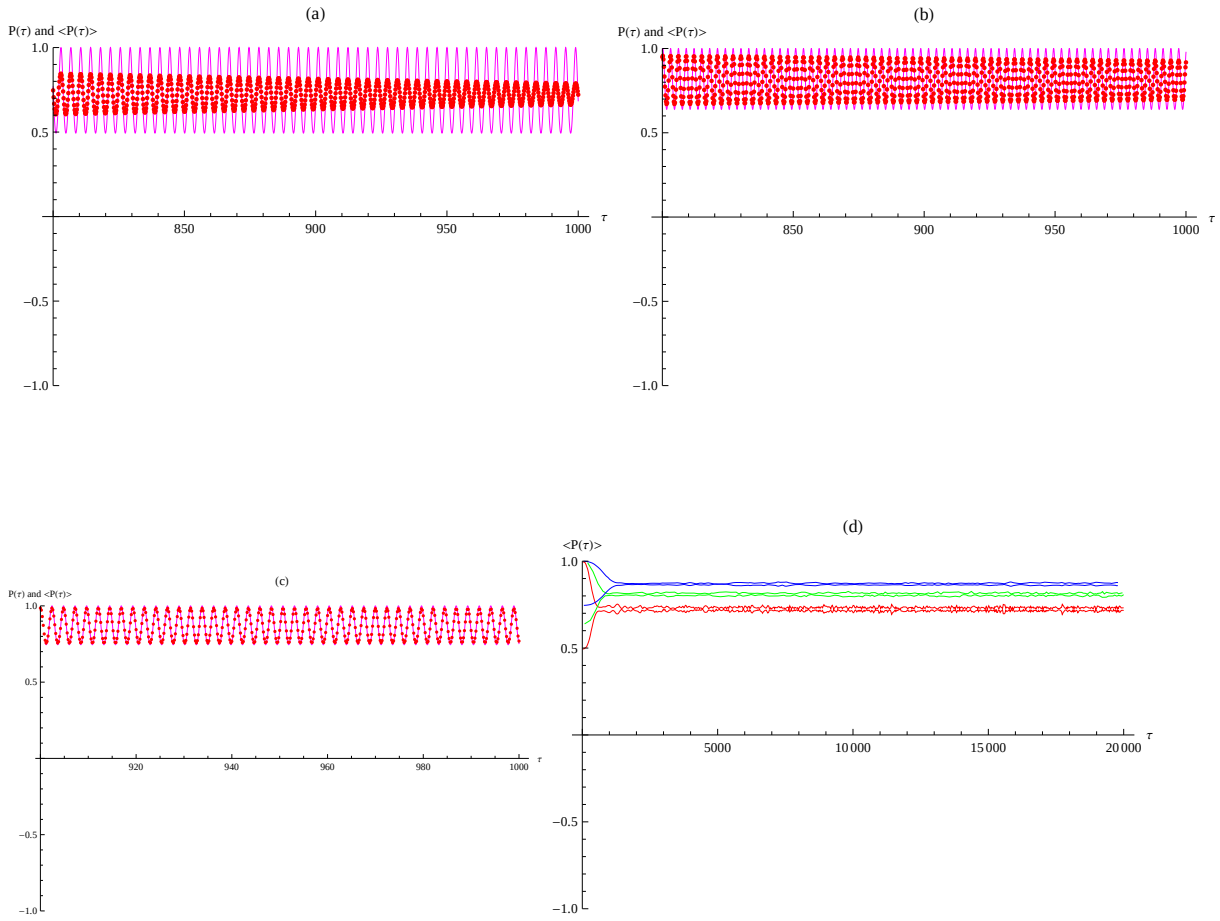

Figure 7: In the graphs, the mean value of probability difference, $< P(\tau) >$, is presented as function of time. In (a),(b),(c) where $\zeta = 1.15, 1.3, 1.5$ respectively, the full line shows the analytical solution of Equation 3.42 while with dotted line are presented the numerical results, for a short time interval. In (d) is presented the envelope of $< P(\tau) >$, for a long time interval where, the (a) case is showed with red color, the (b) case with green and the (c) case with blue. The standard deviation value is $\sigma = 0.1$ while the correlation time is $\tau = 10$

After the advent of system to equilibrium, the various deviations that are observed on the amplitude of $< P(\tau) >$, derived from the numerical calculations of mean value. This divergence is smoothed by increasing the number of repetitions Fig. 8.

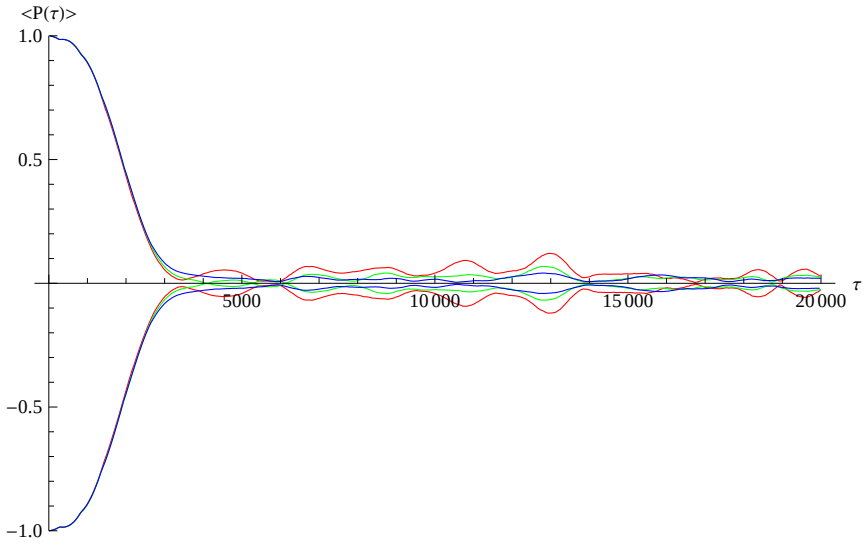

Figure 8: In the graphs, the envelope of mean values of probability differences, $< P(\tau) >$, is presented as function of time. The red area has been taken through 500 repetitions, the green one through 1000 and the blue one through 1500 repetitions.

Thus far, the system has been examined only as regards the nonlinearity, keeping, small standard deviations as well as large correlation times. Furthermore, for a long time interval the mean value of probability difference tend, for all cases of nonlinearity, to a standard value. With that in our mind it would be useful to draw a carve that will reveal the relationship between nonlinearity and $< P(\tau) >$. This effort is disclosed in Fig. 9 . For $\zeta < 1$ the mean value of probability difference remain zero. In the limit, when the nonlinearity is very close to one, is very difficult to have numerical results

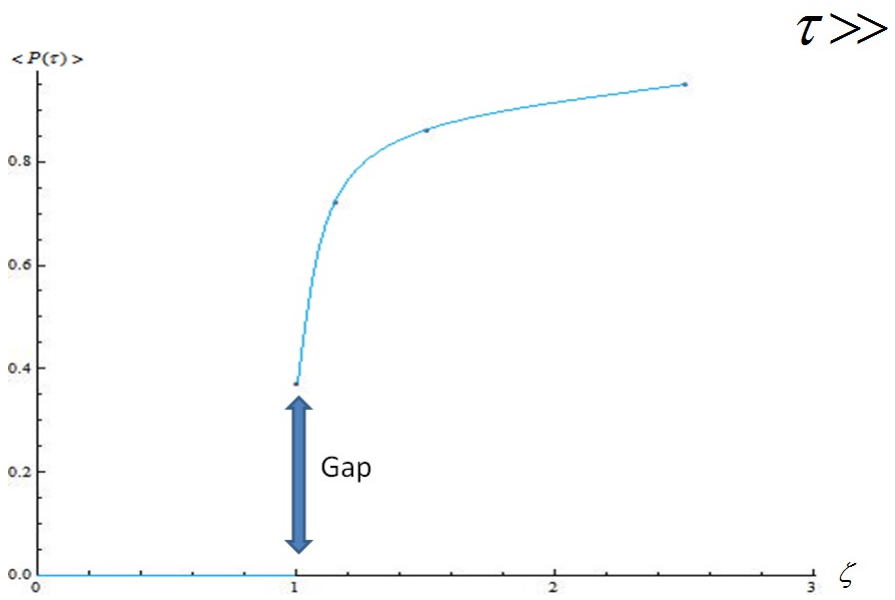

Figure 9: In the graphs, the mean values of probability differences, $< P(\tau) >$, is presented as function of nonlinearity. Time is large enough so the system has ceased to oscillate

because $< P(\tau) >$ growth very fast. In this way, from the numerical inability, in the mean value of probability difference and when $\zeta = 1$ we obtain a gap.Finally, as the nonlinearity takes values larger than one, $< P(\tau) >$ tends very fast to unit.

After the study of system at low stochastic effect, the next step is the consideration of that system through the entire range of correlation times, as well as the standard deviation values by holding a specific nonlinearity.

In the same way as in the linear procedure, between the two parameters, we are keeping the first one fixed (t_c or σ) by changing the second one (σ or t_c) and vice versa.

Keeping the standard deviation constant, the evolution of probability difference, $< P(\tau) >$, as function of t_c and through the progressive of time,

declines. Moreover, the less the value of the correlation time is, the most the declination descends (Fig. 10 and Fig. 11). On the other hand, holding a constant correlation time, $< P(\tau) >$ declines versus time, more sharply, as the value of the standard deviation is getting hayer (Fig.12 and Fig.13)

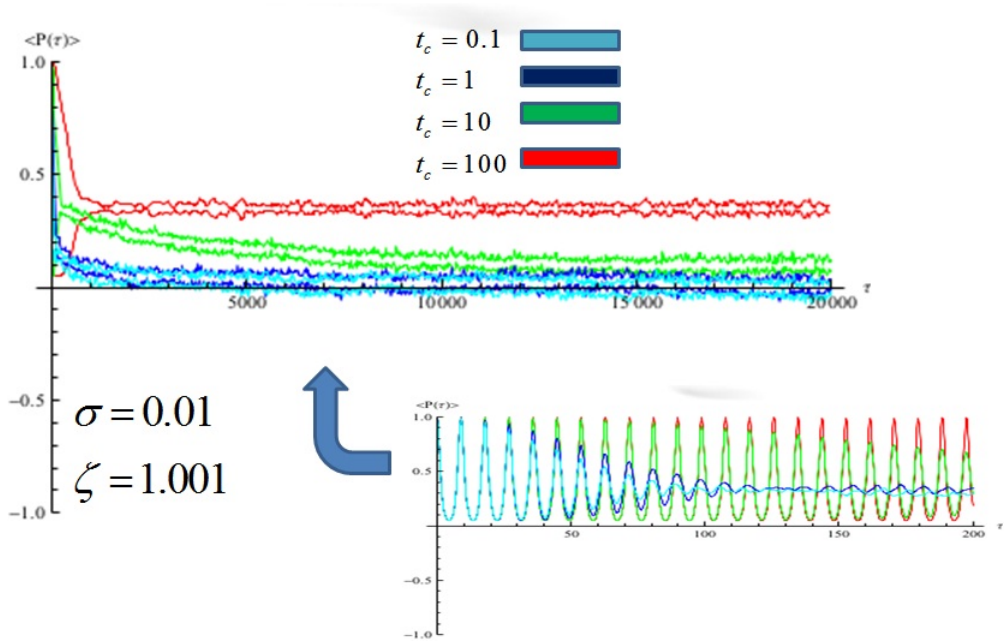

Figure 10: In the graphs, the mean value of probability difference, $< P(\tau) >$, is presented as function of time, keeping the nonlinearity $\zeta = 1.001$ and the standard deviation $\sigma = 0.01$ constant. What is changing is the correlation time. Here, for $t_c = 100, 10, 1, 0.1$, we obtain the above lines from light blue to red color respectively where (a) corresponds to a short time interval and (b) is the envelope of $< P(\tau) >$, for a long time interval

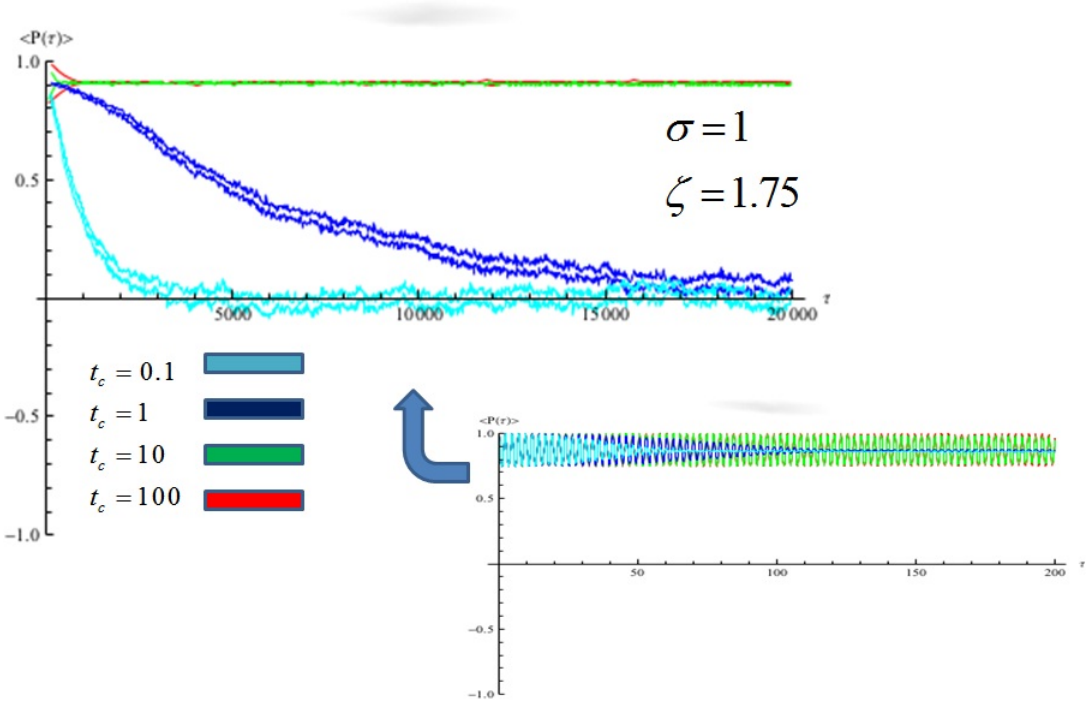

Figure 11: In the graphs, the mean value of probability difference, $< P(\tau) >$, is presented as function of time, keeping the nonlinearity $\zeta = 1.75$ and the standard deviation $\sigma = 1$ constant. What is changing is the correlation time. Here, for $t_c = 100, 10, 1, 0.1$, we obtain the above lines from light blue to red color respectively where (a) corresponds to a short time interval and (b) is the envelope of $< P(\tau) >$, for a long time interval.

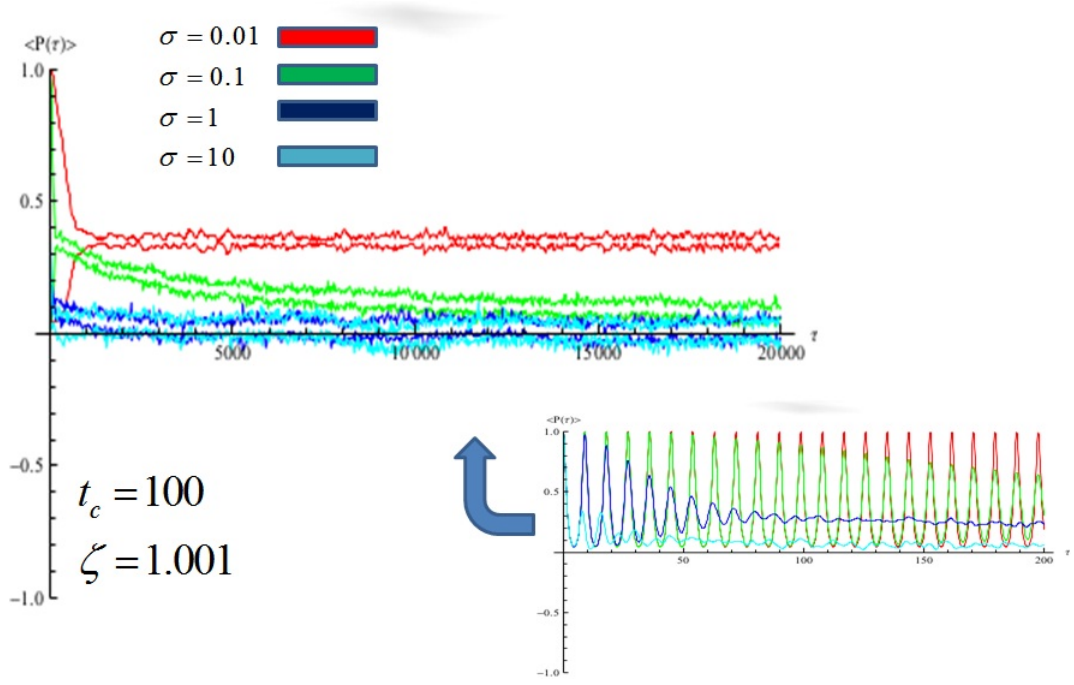

Figure 12: In the graphs, the mean value of probability difference, $< P(\tau) >$, is presented as function of time, keeping the nonlinearity $\zeta = 1.001$ and the correlation time $t_c = 100$ constant. What is changing is the standard deviation. Here, for $\sigma = 0.01, 0.1, 1, 10$ we obtain the above lines, from red to light blue color respectively, Here, for $t_c = 100, 10, 1, 0.1$, we obtain the above lines from light blue to red color where (a) corresponds to a short time interval and (b) is the envelope of $< P(\tau) >$, for a long time interval.

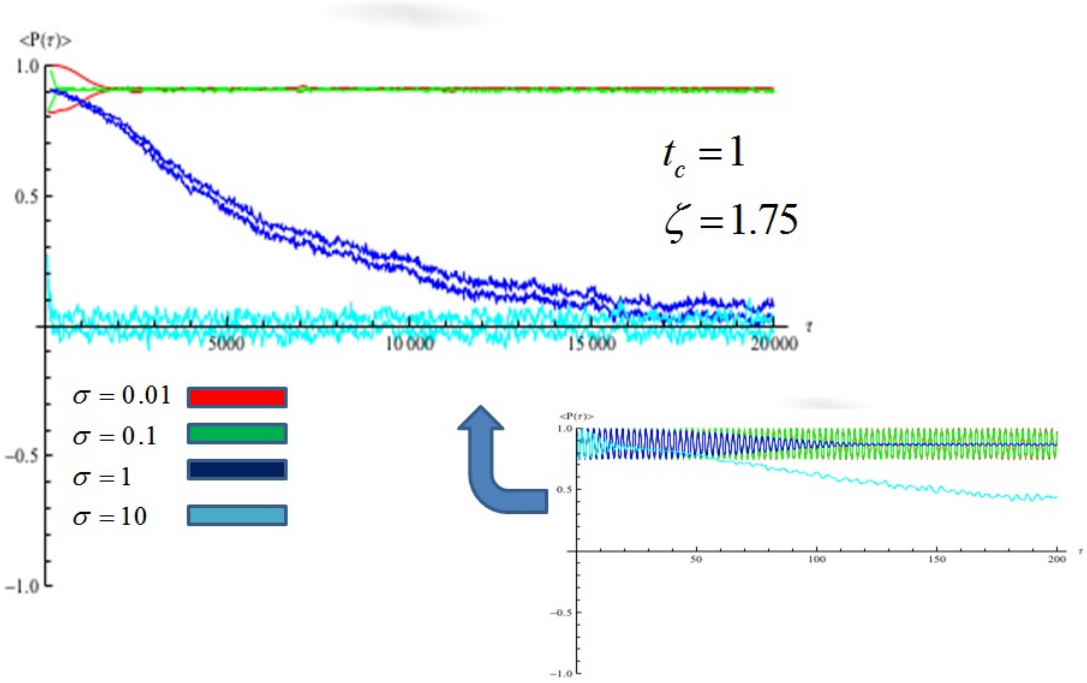

Figure 13: In the graphs are presented the mean value of probability difference, $< P(\tau) >$ as function of time, keeping the nonlinearity $\zeta = 1.75$ and the correlation time $t_c = 1$ constant. What is changing is the standard deviation.Here, for $t_c = 100, 10, 1, 0.1$, we obtain the above lines from light blue to red color where (a) corresponds to a short time interval and (b) is the envelope of $< P(\tau) >$, for a long time interval.

As emphasized in the linear case, the function of the probability difference, under stochastic processes, tends to zero. The only that is defined by correlation time and standard deviation is the time frame of such tendency. In the presence of nonlinearity, no large differences arise . The truth is that, between the last one and this of stochastic processes, a competition is appear. However, after a interval time, the outcome is the same. The "force" of nonlinearity, is trying to keep the system in an "equilibrium" value, but not forever. After a certain, interval time, the probability difference tends again to zero.

5 Diffusion and Hypertransport

The Mean Square Displacement (mean square displacement is the name of the second moment for a given statistical problem) is a way to quantify the electronic propagation. The Mean Square Displacement (MSD) is a function of time, and is given by

$$< n^2(\tau) = \sum_{-\infty}^{\infty}(n - n_0)^2|c_n(\tau)|^2 \tag{5.1}$$

where $(n-n_0)^2$ is the deviation from the site that the electron (or excitation) was placed initially,n_0, and $|c_n(\tau)|^2$ is the probability of finding the electron in the n^{th} site. The summation is over all sites in the lattice. As the electron propagates from the site where it is initially placed to the boundary, the Mean Square Displacement grows. In an infinite lattice, where the electron propagates for infinite time, the Mean Square Displacement goes to infinity.

In the case of dimer we obtain

$$< n^2(\tau) >= |c_2(\tau)|^2 \tag{5.2}$$

and with the advent of stochastic processes it is necessary to receive the mean value

$$<< n^2(\tau) >>=< |c_2(\tau)|^2 > \tag{5.3}$$

In our graphs we are investigate the mean value of probability difference. Beyond the oscillatory behaviour, we observe a kind of diffusion. In all cases, the envelope of $< P(\tau) >$, after a long time interval, move to zero. The mean of that behaviour is the increase, after each oscillatory period, of probability to find the particle on the second site. If we want to calculate the growth rate of $< |c_2(\tau)|^2 >$, we must use the probability conservation $|c_1(\tau)|^2 + |c_2(\tau)|^2$. With that help, we are able to get a graph where we put $2 < |c_2(\tau)|^2 >$ at vertical axes and we the time at horizontal ones. Furthermore, if we want

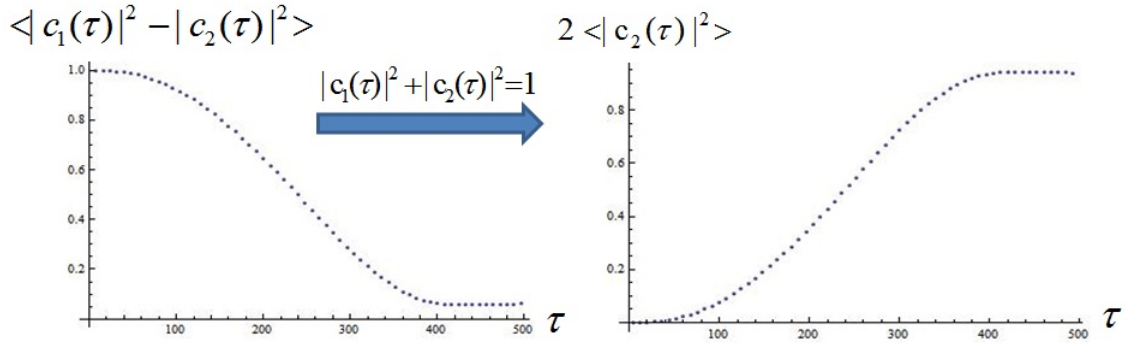

Figure 14: In the first graph is presented a random curve as the mean value of probability difference, $< P(\tau) >$. In the second graph, with the inversion of the first one, we have constructed the mean value of probability to find the particle on the second site

the range of $2 < |c_2(\tau)|^2 >$ to be start from zero we must reverse all the graph (see Fig. 14).

Diffusion is often described by a power law $< n^2(\tau) > \sim D\tau^a$, where D is the diffusion coefficient and τ is the elapsed time. In a typical diffusion process, $a = 1$. If $2 > a > 1$ the phenomenon is called super-diffusion. If $a < 1$, the particle undergoes sub-diffusion. If $a = 2$ we have a ballistic motion and if $a > 2$ the motion is called hypertransport.

Now, if we admit that the rate of diffusion is actually described by $< |c_2(\tau)|^2 >$, then the total picture reads as follows.

With the advent of a large stochastic effect the system behaves like sub-diffusion. The diffusion comes as a limiting case when the correlation time get large value (see Fig. 15). In contrast, if we put together, a low stochastic effect with nonlinearity, we obtain a hypertransport phenomenon. Again, the ballistic transport can be possible when nonlinearity approaches marginally the unit (see Fig.16)

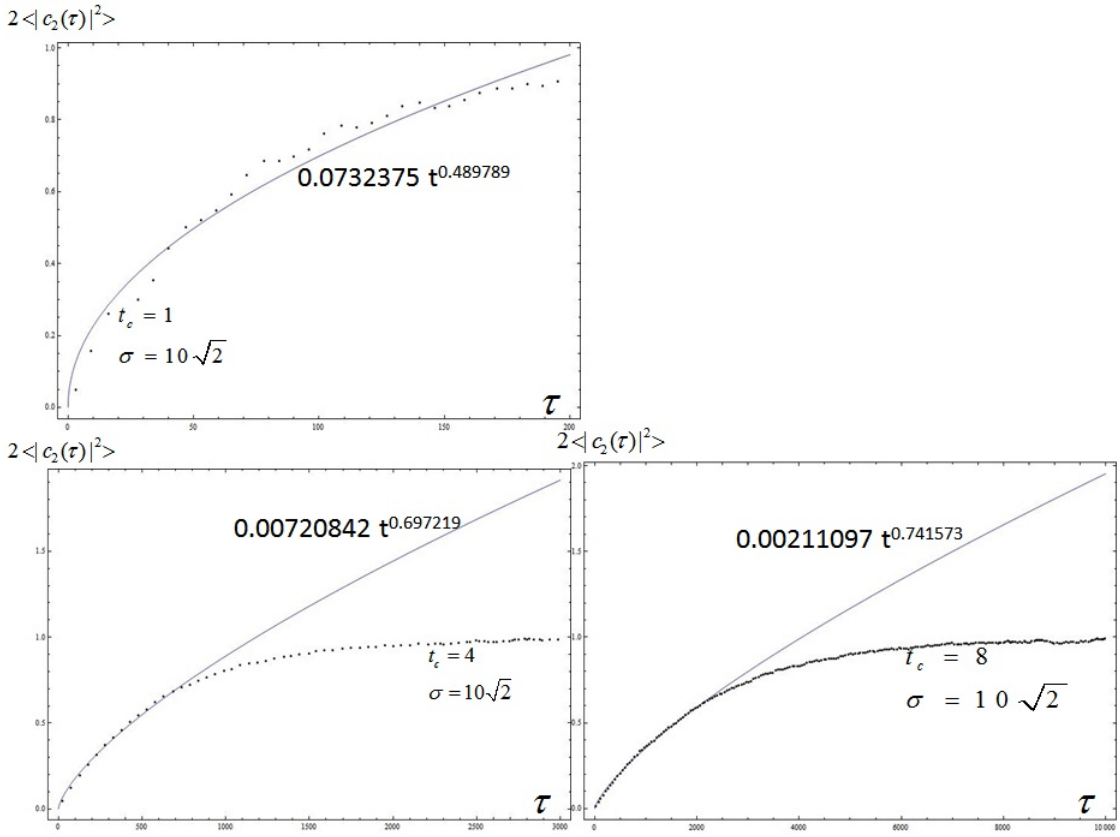

Figure 15: In the graphs are presented the mean value of probability to find the particle on the second site, $< |c_2(\tau)|^2 >$ as function of time for different values of correlation time. With dotted line are presented the numerical results while the full line shows the fit

6 CONCLUSIONS

In the linear case, the interval time, before $< P(\tau) >$ reaches the zero value, has been determined by two parameters. They are the correlation time and the standard deviation.

The mean value of probability difference declines versus time, more sharply, the higher the value of the standard deviation is. In contrast, through the

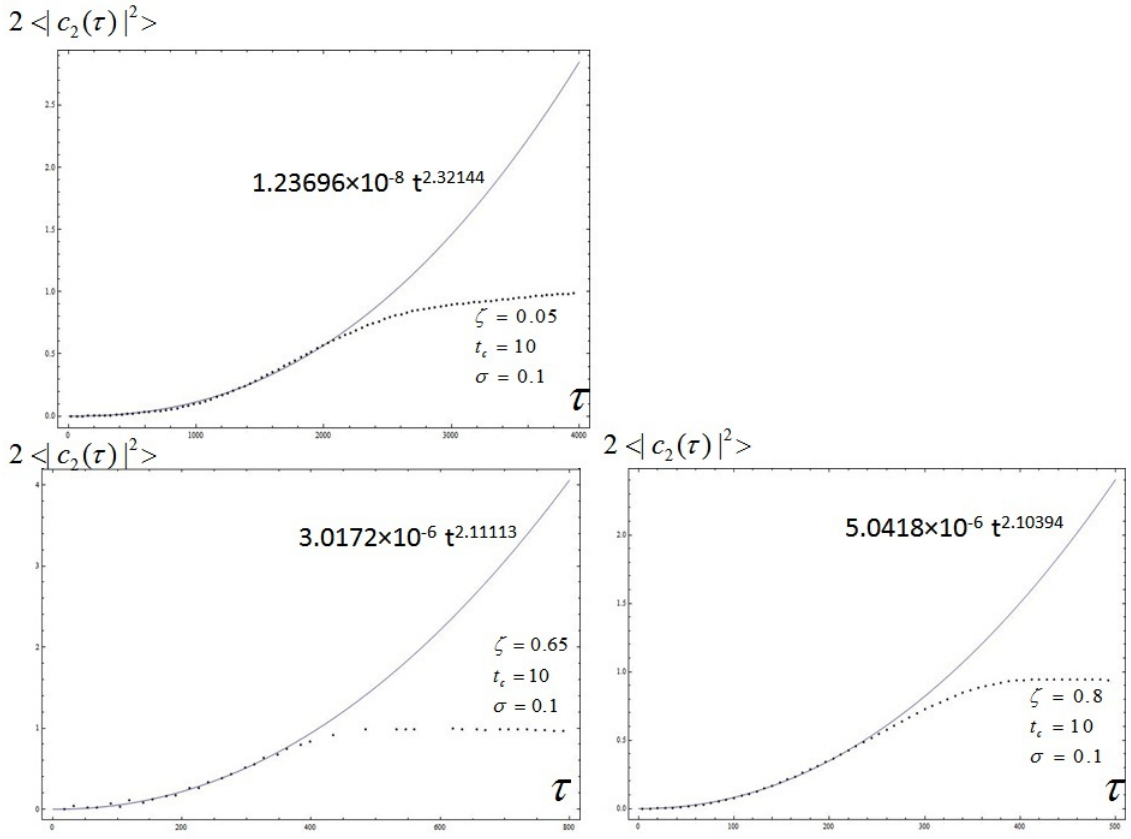

Figure 16: In the graphs are presented the mean value of probability to find the particle on the second site, $< |c_2(\tau)|^2 >$ as function of time for different values of nonlinearity. With dotted line are presented the numerical results while the full line shows the fit

progressive of time, the less the value of the correlation time is, the most the declination of $< P(\tau) >$ descends.

Before the advent of stochastic processes , the nonlinearity surfaced hosts of properties. For $\zeta < 1$ the evolution of $< P(\tau) >$ take place on both the positive and negative axis while, for $\zeta > 1$, is restricted only to the positive axis. It seems that, with nonlinearity been increased, the mean value of

the probability difference, is descending quickly, to an "equilibrium", time average of $< P(\tau) >$.

When the nonlinearity is greater than one, the evolution of system takes place only in one site, where the mean value of the probability difference is positive. As the nonlinearity grows, the $< P(\tau) >$, after an oscillatory behaviour, tends to one.

After the advent of stochastic processes, the main conclusion is just one. The mean value of function of the probability difference , under stochastic processes and after an interval time , tends to zero. This situation takes place for any value of nonlinearity. The "force" of nonlinearity trying to keep the system in an "equilibrium" value. More precisely, the increase of nonlinearity keep the system in that special value, in a more time interval. However, under stochastic processes constraint, the probability difference tends again to zero.

It seems that when stochastic processes takes place we obtain a sub-diffusion behaviour. Hypertranspor phenomenon can be possible with the entrance of nonlinearity.

Finally, what we need to emphasize is the identification of numerical results with the analytical one. The later, has been clear for both linear and nonlinear case. These results confirm the numerical calculations validity.

APPENDIX

7 The nonlinear Schrödinger equation

It is often convenient to write the solution of a linear wave problem in the form

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(k)e^{i(kx-\omega t)}dk \tag{7.1}$$

where $F(k)$ is the Fourier transform of $u(x,0)$ and ω is relate to k through the dispersion relation $\omega = \omega(k)$. Unless $\omega = k$, each component in Equation 7.1 travels at different (ω/k), and the wave disperses.

A wave packet is a special form of Equation 7.1 with the Fourier components lying to some propagation number (k_0) and the corresponding frequency(ω_0). In other words, $F(k)$ has its maximum value at $k = k_0$, falling rapidly as $|k - k_0|$ increases and allowing the dispersion relation to be expanded as a power series about k_0.

With the notation

$$\omega = \omega_0 + b_1(k - k_0) + b_2(k - k_0)^2 \tag{7.2}$$

Equation 7.1 becomes

$$u(x,t) = e^{i(k_0x-\omega_0t)}\frac{1}{2\pi}\int_{-\infty}^{\infty} F(k)e^{i\{(k-k_0)x-b_1(k-k_0)t-b_2(k-k_0)^2t\}}dk \tag{7.3}$$

where the factor $e^{i(k_0x-\omega_0t)}$ is a carrier wave with velocity $u_c = \frac{\omega_0}{k_0}$. Riding over the carrier is an envelope wave

$$\phi(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(k+k_0)e^{i\{kx-b_1kt-b_2k^2t\}}dk \tag{7.4}$$

where the variable of integration has been changed from k to $k = k - k_0$. Taking the time derivative of Equation 7.4, one finds

$$\frac{\vartheta\phi}{\vartheta t} = \frac{1}{2\pi}\int_{-\infty}^{\infty} -i(b1k + b_2k^2)F(k+k_0)e^{i\{kx - b_1kt - b_2k^2t\}}dk \tag{7.5}$$

$$\frac{\vartheta\phi}{\vartheta t} = -b_1\frac{\vartheta\phi}{\vartheta x} + ib_2\frac{\vartheta^2\phi}{\vartheta x^2} \tag{7.6}$$

thus

$$i(\frac{\vartheta\phi}{\vartheta t} + b_1\frac{\vartheta\phi}{\vartheta x}) + b_2\frac{\vartheta^2\phi}{\vartheta x^2} = 0 \tag{7.7}$$

Up to this point, the discussion has remained within the realm of linear theory, but we now consider how a small amount of nonlinearity will alter Equation 7.7 . If a is the local amplitude of the wave envelope, the lowest order contribution to the dispersion relation will be proportional to a^2. First-order terms in a do not appear because this would imply dependence of envelope dynamics on the sign of the carrier wave, which change each half cycle of the carrier frequency. From equation 7.7, the dispersion relation for the envelope of a linear packet is

$$\omega = b_1k + b_2k^2 \tag{7.8}$$

Noting the square of the amplitude $a^2 = |\phi|^2$, it follows that

$$i(\frac{\vartheta\phi}{\vartheta t} + b_1\frac{\vartheta\phi}{\vartheta x}) + b_2\frac{\vartheta^2\phi}{\vartheta x^2} + \chi|\phi|^2\phi = 0 \tag{7.9}$$

where χ is a real number, the nonlinear dispersion becomes

$$\omega = b_1k + b_2k^2 - \chi a^2 \tag{7.10}$$

Equation 7.9 is the nonlinear SchrÃűdinger equation, which has the following properties

1. Describe the propagation of an envelope wave, riding over a carrier. 2. If the envelope varies sufficiently slowly with x and is of small enough amplitude, then the last two terms on the left hand site can be neglected, and the envelope wave moves with the group velocity

$$u_g = b_1 = \frac{\vartheta\omega}{\vartheta k}|_{k=k_0} \tag{7.11}$$

3. The term $b_2(\vartheta^2\phi/\vartheta x^2)$ introduces wave dispersion into the problem at the lowest level of approximation. Similarly, the term $\chi|\phi|^2\phi$ introduces nonlinearity at the lowest level of approximation.

7.1 Derivation of the discrete nonlinear Schrödinger equation

Our starting point for the derivation of the DNLS equation will be the continuum nonlinear Schrödinger equation for the wave function ψ in the presence of a periodic potential of the form

$$i\frac{\vartheta\psi}{\vartheta t} = -\frac{\vartheta^2\psi}{\vartheta x^2} + V(x)\psi + \chi(|\psi|^2)\psi \tag{7.12}$$

where $V(x)$ is a periodic potential and χ is the nonlinear parameter

We start by considering the linear eigenvalue problem

$$-\frac{d^2\phi_{k,a}}{dx^2} + V(x)\phi_{k,a} = E_a(k)\phi_{k,a} \tag{7.13}$$

where $\phi_{k,a}$ has BlochFloquet function (BFs) $\phi_{k,a} = e^{ikx}u_{k,a}(x)$, with $u_{k,a}(x)$ periodic with period L; a labels the energy bands $E_a(k)$. It is well know that $E_a(k+2/L) = E_a(k)$. The energy can therefore be represented as a Fourier series

$$E_a(k) = \sum_n \tilde{\omega}_{n,a}e^{iknL}, \tilde{\omega}_{n,a} = \tilde{\omega}_{-n,a} = \tilde{\omega^*}_{n,a} \tag{7.14}$$

where an asterisk stands for complex conjugation and

$$\tilde{\omega}_{n,a} = \frac{L}{2\pi} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} E_a(k) e^{iknL} dk \tag{7.15}$$

The BFs constitute an orthogonal bases; instead of that basis, we will use the Wannier function (WF) one. The WF centered around the position nL (n is an integer) and corresponding to the band a is defined as

$$w_a(x - nL) = \sqrt{\frac{L}{2\pi}} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} \phi_{k,a}(x) e^{iknL} dk \tag{7.16}$$

Conversely,

$$\phi_{k,a}(x) = \sqrt{\frac{L}{2\pi}} \sum_{n=-\infty}^{\infty} w_{n,a}(x) e^{iknL} \tag{7.17}$$

The WFs also form a complete orthonormal (with respect to both n and a) set of functions,

$$\sum_{n,a} w^*_{n,a}(x) w_{n',a'}(x) dx = \delta_{aa'} \delta_{nn'} \tag{7.18}$$

$$\int_{-\infty}^{\infty} w^*_{n,a}(x) w_{n,a}(x') dx = \delta(x - x') \tag{7.19}$$

witch, by properly choosing the phase of the BFs in 7.16, can by made real and exponentially decaying at infinity. We therefore assume this chose: $w_{n,a}(x) = w^*_{n,a}(x)$. At the heart of the derivation of the DNLS equation lies the decomposition of the solution of 7.12 in the basic of WFs (given the completeness of this basis)

$$\psi(x,t) = \sum_{n,a} c_{n,a}(t) w_{n,a}(x) \tag{7.20}$$

This decomposition is then substituted in 7.12 yielding

$$i\frac{dc_{n,a}}{dt} = \sum_{n1} c_{n1,a}\tilde{\omega}_{n-n1,a} + \chi \sum_{a1,a2,a3} \sum_{n1,n2,n3} {c^*}_{n1,a1} c_{n2,a2} c_{n3,a3} W^{nn1n2n3}_{aa1a2a3} \quad (7.21)$$

where

$$W^{nn1n2n3}_{aa1a2a3} = \int_{-\infty}^{\infty} w_{n,a} w_{n1,a1} w_{n2,a2} w_{n3,a3} dx \quad (7.22)$$

are overlapping matrix elements. The expression $W^{nn1n2n3}_{aa1a2a3}$ is symmetric with respect to all permutations within the groups of indices $(a, a1, a2, a3)$ and $(n, n1, n2, n3)$. Eq.7.20 can be viewed as a vector form of the DNLS equation for $c_n = col(c_{n1}, c_{n2}, ...)$ with non-nearest-neighbour interactions in its general form. A key question then concerns the potential simplifications and the conditions under which it can be reduced to single-component DNLS equation.

For sufficiently rapid decay of the Fourier coefficients in 7.15 and $|\tilde{\omega}_{1,a}| >> |\tilde{\omega}_{n,a}|, n > 1$ the non-nearest-neighbour coupling terms can be neglected in the linear part of Eq.7.20, leading to a dynamical model accounting solely for nearest-neighbour interactions.

Secondly, since $w_{n,a}(x)$ is localized and centred around $x = nL$, one can assume that in some case among all the coefficients $W_{aa1a2a3}$ those with $n = n1 = n2 = n3$ are dominate and other terms can be neglected, since they are exponentially weaker. Then, one arrives at the equation

$$i\frac{dc_{n,a}}{dt} = \tilde{\omega}_{0,a} c_{n,a} + \tilde{\omega}_{1,a}(c_{n-1,a} + c_{n+1,a}) + \chi \sum_{a1,a2,a3} W^{nnnn}_{aa1a2a3} c^*_{n,a1} c_{n,a2} c_{n,a3} \quad (7.23)$$

which becomes the tight-binding DNLS model

$$i\frac{dc_{n,a}}{dt} = \tilde{\omega}_{0,a} c_{n,a} + \tilde{\omega}_{1,a}(c_{n-1,a} + c_{n+1,a}) + \chi W^{nnnn}_{1111} |c_{n,a}|^2 c_{n,a} \quad (7.24)$$

by restricting consideration only to the band a. One of the advantages of this derivation is that it show directly how to generalize the single band approximation, both in the direction of including additional bands when relevant(i.e. when the inter-band coupling terms are comparable to the intra-band ones) and also toward that of including additional neighbours within a band when $\tilde{\omega}_{n,a}$ for $n > 1$ become sizeable with respect to $\tilde{\omega}_{1,a}$. Both of these properties are determined by the linear properties of the model, which yields $\tilde{\omega}_{n,a}$ and $w_{n,a}(x)$ and the specific form of the nonlinearity (which determines the particular form of the overlap coefficients to be compared between bands and between sites).

7.2 Numerical Integration (Heun Method)

We assume that we have to solve the differential equation

$$\dot{x} = f(x) + \xi(t) \tag{7.25}$$

where

$$P(\xi) = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{-x^2}{2\sigma}} \tag{7.26}$$

have a Gaussian distribution with

$$< \xi >= 0 \tag{7.27}$$

$$< \xi\xi' >= 2D\delta(t - t') \tag{7.28}$$

In integral form

$$\int_t^{t+h} dx = \int_t^{t+h} f(x(t'))dt' + \int_t^{t+h} \xi(t')dt' \tag{7.29}$$

For h small enough

$$x(t+h) = x(t) + f(x(t)) + W \tag{7.30}$$

where

$$W = \int_t^{t+h} \xi(t')dt' \tag{7.31}$$

is a sum of Gaussian distributions having the same distribution form with

$$< W >= 0 \tag{7.32}$$

$$< w^2 >= \int_t^{t+h} dt' \int_t^{t+h} dt' < \xi(t')\xi(t'') >= 2Dh \tag{7.33}$$

As we can see $\sigma^2 =< W > - < W^2 >= 2Dh \Rightarrow D = \sigma^2/2h$.

Defining $W = \sqrt{2Dh}Y$, where Y is a function with, again, Gaussian distribution , equation 7.30 becomes

$$x(t+h) = x(t) + f(x(t))h + \sqrt{2Dh}Y \tag{7.34}$$

Eventually, we define Heun method as

$$x(t+h) = x(0) + \sqrt{2Dh}Y + \frac{h}{2}(f(x(t)) + f(\phi)) \tag{7.35}$$

where

$$\phi = x(t) + f(x(t))h + \sqrt{2Dh}Y \tag{7.36}$$

7.3 Exponentially distributed noise

A noise force with the δ correlation 3.3 is called white noise, because the special distribution which is given by Fourier transform is then independent of the frequency ω . If the stochastic forces are not δ correlated, one use

the term coloured noise. In further detail we assume a random variable $\xi(t)$. The Fourier transform is

$$\tilde{\xi} = \int_{-\infty}^{\infty} e^{-i\omega t}\xi(t)dt \tag{7.37}$$

which is also a random variable.

$$< \tilde{\xi}(\omega)\tilde{\xi^*}(\omega') >= \int\int e^{-i\omega t+i\omega t'} < \xi(t)\xi(t') > dtdt' \tag{7.38}$$

Introducing the new variables $\tau = t - t'$ and $t_0 = (t' + t)/2$ we have

$$< \tilde{\xi}(\omega)\tilde{\xi^*}(\omega') >= \int_{-\infty}^{infty} e^{(-i(\omega-\omega')}dt_0 \int_{-\infty}^{\infty} e^{-i(\omega'+\omega)\tau/2} < \xi(\tau)\xi^*(0) > d\tau \tag{7.39}$$

$$\Longrightarrow < \tilde{\xi}(\omega)\tilde{\xi^*}(\omega') >= \pi\delta(\omega - \omega')S(\omega) \tag{7.40}$$

where

$$S(\omega) = 2\int_{-\infty}^{\infty} e^{-i\omega\tau} < \xi(\tau)\xi^*(0) > d\tau \tag{7.41}$$

is the special distribution. For $< \xi(\tau)\xi^*(0) >= D\delta(\tau)$ the above equation becomes

$$S(\omega) = 2D\int_{-\infty}^{\infty} e^{-i\omega\tau}\delta(\tau)d\tau = 2D = constant \tag{7.42}$$

For the noise used in our problem 3.1 we can take a decision through the following calculations.

First, we try to solve the differential equation 3.1. With a change of variable $\epsilon(t) = g(t)Y(t)$ and after some calculations, we obtain

$$\epsilon(t) = \epsilon(0)e^{-\gamma t} + \int_0^t e^{-\gamma(t-t')}\Gamma(t')dt' \tag{7.43}$$

where $\Gamma(t)$ has the properties 3.2, 3.3 with $\gamma = 1/t_c$. With these informations we can evaluate the mean value as well as the mean square value of $\epsilon(t)$ as follows

$$< \epsilon(t) >=< \epsilon(0)e^{-\gamma t} > + \int_0^t e^{-\gamma(t-t')} < \Gamma(t') > dt' \tag{7.44}$$

With the initial condition $\epsilon(0) = 0$ and taking account the property 3.2 we obtain that $< \epsilon(t) >= 0$. For the mean square value of ϵ more calculations are needed. Initially, for $\epsilon(0) = 0$ we have

$$< \epsilon(t_1)\epsilon(t_2) >= \int_0^{t_1} \int_0^{t_2} e^{-\gamma(t_1+t_2-t_1'-t_2')} < \Gamma(t_1')\Gamma(t_2') > dt_1' dt_2' \tag{7.45}$$

$$= D\gamma^2 \int_0^{t_1} \int_0^{t_2} e^{-\gamma(t_1+t_2-t_1'-t_2')}\delta(t_1' - t_2')dt_1' dt_2' \tag{7.46}$$

To calculate the double integral, we integrate over t_2' first. The integration over t_1' then runs only from 0 to t_2 or t_1 is less. We therefore have

$$< \epsilon(t_1)\epsilon(t_2) >= D\gamma^2 \int_0^{min(t_1,t_2)} e^{-\gamma(t_1+t_2-2t_2')}dt_2' \tag{7.47}$$

$$= \frac{D\gamma}{2}(e^{-\gamma|t_1-t_2|} - e^{-\gamma(t_1+t_2)}) \tag{7.48}$$

For large t_1 and t_2 , the energy correlation function is only dependent of the time difference

$$< \epsilon(t_1)\epsilon(t_2) >= \frac{D\gamma}{2}e^{-\gamma|t_1-t_2|} \tag{7.49}$$

Putting this result into the integral of the spectral density we can clearly see that $S = S(\omega)$.

Remarks on the Spectral Density:

The field strength $E(t)$ in a optical wave may be considered as a random variable. If such a wave goes through a prism, the prism separates the

different Fourier components $\tilde{E}(\omega)$ of the incoming wave, and the intensity measured in a spectrometer is given by $\tilde{E}(\omega)\tilde{E}*(\omega)$. For infinitely long observation this intensity is infinite. For large but finite observation times T the intensity is given by the spectral density $S(\omega)$ times the observation time T.

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