MIDDLE EAST TECHNICAL UNIVERSITY
DEPARTMENT OF PHYSICS

50 years in research & education

PHYS400 Final Report

Prepared by

Rafet KAVAK

2166783

Project Title: *A new real-time technique to study chaotic dynamics at quantum level*

Submission Date: *12/07/2021*

Supervisor: *Seçkin KÜRKÇÜOĞLU*

e-Mail: *kseckin@metu.edu.tr*

Table of Contents

1) Introduction

"In this work, the article "Real-time dynamics of matrix quantum mechanics beyond the classical approximation [1]" was followed to gain insight into how new real-time techniques can be developed to study chaotic dynamics at the quantum level. Before mentioning what has been done, a brief motivation will be presented underlying the article. Then, the conducted study within the scope of the PHYS400 course will be summarized before the method section."

Thermalization, the relaxation of a system to a uniform temperature, of highly interacting quantum systems, is one of the most challenging problems in current heavy-ion physics [2-5]. From thermalization of the quark-gluon plasma in heavy-ion collisions to inflation of the Universe, physicists have several thoughts to describe the phases of the early Universe. In the existence of large field strengths, i.e., large quantum occupation numbers and small coupling constants, the classical equations of motion can be used [6, 7]. In the dilute plasma regime with small quantum occupation numbers, kinetic theory description can be used [8]. The intermediate regime between these stages is crucial for matching the early-time strongly non-equilibrium evolution and the late-time hydrodynamic behaviour [2, 9]. To examine this intermediate regime, the following Hamiltonian (1) was considered which is classically chaotic and features thermalization [10].

$$H = \frac{1}{2}\sum_{i} TrP_i^2 - \frac{1}{4}\sum_{i,j} Tr\left[X_i, X_j\right]^2 \tag{1}$$

The studies that have previously conducted this kind of Hamiltonians were based upon the classical mechanics approximation. In this project, the Gaussian state approximation will be used to analyze how the classically chaotic Hamiltonian (1) might be affected by the quantum effects.

In the PHYS400 course perspective, in order to find the quantum mechanical time evolution of a system for a given Hamiltonian, the Heisenberg equations for the canonically conjugate operators of that Hamiltonian were found at first. Then, by averaging these equations with respect to a density matrix (represented by the Gaussian state Wigner function), the equations of motion for the expectation values of canonically conjugate operators and the expectation values of newly emerged operator products as a consequence of Gaussian state approximation were obtained (which are Gaussian wave packet centers and dispersions respectively). After solving the complete system of equations numerically, the time evolutions of phase space variables obtained from the Gaussian state approximation and obtained from classical equations of motion were compared.

2) Method

In this section, the method of the Gaussian state approximation will be discussed.

To analyze the quantum mechanical time evolution of a system, the complete system of equations must be determined. For this purpose, the Gaussian state approximation will be applied on a Hamiltonian (2), the reduced version of Yang-Mills type Hamiltonians in Eq. 1., to obtain these equations. Notice that this Hamiltonian still shows the chaotic characteristic.

$$H = \frac{p_x^2}{2} + \frac{p_y^2}{2} + \frac{x^2 y^2}{2} \tag{2}$$

First of all, the Heisenberg equations for the canonically conjugate operators $\hat{x}, \hat{y}, \hat{p}_x, \hat{p}_y$ will be obtained for a given Hamiltonian (2). Then the equations of motion for the expectation values of these operators can be obtained according to a density matrix $\rho(\xi)$ where $\xi = \{x, y, p_x, p_y\}$. After trying to take the expectation values of these operators, resulting equations of motion will contain $\langle \hat{x}\hat{y}^2 \rangle$ types of expectation values, so the calculations will continue forever. These endless consecutive equations can be truncated by approximating the density matrix $\rho(\xi)$ using the most general time-dependent Gaussian function. In this way, the expectation values that consist of multiple momentum and coordinate operators can be denoted as the coordinates of the centers and dispersion of a wave packet. For this purpose, it is more suitable to use the Wigner function to characterize the most general Gaussian state

$$\rho(\xi) = \mathcal{N} \exp\left(-\frac{1}{2} (\xi - \bar{\xi}) \Sigma^{-1} (\xi - \bar{\xi}) \right) \tag{3}$$

where $\xi = \{x, y, p_x, p_y\}$ is the vector consists of phase space variables, and the parameter Σ can be defined as

$$\Sigma_{ab} = \langle\langle \xi_a \xi_b \rangle\rangle \equiv \langle \frac{\hat{\xi}_a \hat{\xi}_b + \hat{\xi}_b \hat{\xi}_a}{2} \rangle - \langle \hat{\xi}_a \rangle \langle \hat{\xi}_b \rangle \tag{4}$$

where $\bar{\xi}_a = \langle \hat{\xi}_a \rangle$ describes the center of the wave packet and $\langle\langle \xi_a \xi_b \rangle\rangle$ describes the wave packet dispersion.

Let us obtain the Heisenberg equations for the operators now. To begin with, it is helpful to remember the Heisenberg equations

$$\frac{d}{dt} A_H(t) = \frac{i}{\hbar} [H_H, A_H(t)] + \left(\frac{\partial A_S}{\partial t} \right)_H \tag{5}$$

where $H_H, A_H(t)$ are two operators. Notice that “H” and “S” labels are for Heisenberg and Schrödinger picture, respectively. Then for the position operator, let us obtain the Heisenberg equation.

$$\frac{d\hat{x}}{dt} = \frac{i}{\hbar} [\hat{H}, \hat{x}] + \frac{\partial \hat{x}}{\partial t} \tag{6}$$

where $\frac{\partial \hat{x}}{\partial t} = 0$ because there is no explicit time dependence. It is also better to remember the basic commutator identities, which can be shown in Equations 7,8.

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B} \tag{7}$$

$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C} \tag{8}$$

Then Eq. 6 becomes

$$\frac{d\hat{x}}{dt} = \frac{i}{\hbar}\left[\frac{\hat{p}_x^2}{2}, \hat{x}\right] = \frac{i}{\hbar}\left(\frac{\hat{p}_x}{2}[\hat{p}_x, \hat{x}\,] + [\hat{p}_x, \hat{x}\,]\frac{\hat{p}_x}{2}\right) \tag{9}$$

$$\frac{d\hat{x}}{dt} = \frac{i}{\hbar}\hat{p}_x[\hat{p}_x, \hat{x}\,] \quad where \quad [\hat{x}, \hat{p}_x] = i\hbar \tag{10}$$

$$[\hat{p}_x, \hat{x}] = [\hat{x}, \hat{p}_x] = -i\hbar \tag{11}$$

$$\frac{d\hat{x}}{dt} = \frac{i}{\hbar}\hat{p}_x(-i\hbar) = \hat{p}_x \tag{12}$$

Finally,

$$\boxed{\partial_t \hat{x} = \hat{p}_x} \tag{13}$$

Likewise,

$$\boxed{\partial_t \hat{y} = \hat{p}_y} \tag{14}$$

For the momentum operators,

$$\frac{d\hat{p}_x}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{p}_x] + \frac{\partial \hat{p}_x}{\partial t} \tag{15}$$

where $\frac{\partial \hat{p}_x}{\partial t} = 0$ because there is no explicit time dependence. Then,

$$\frac{d\hat{p}_x}{dt} = \frac{i}{\hbar}\left[\frac{\hat{x}^2\hat{y}^2}{2}, \hat{p}_x\right] = \frac{i}{\hbar}\frac{\hat{y}^2}{2}[\hat{x}^2, \hat{p}_x] \tag{16}$$

$$\frac{d\hat{p}_x}{dt} = \frac{i}{\hbar}\frac{\hat{y}^2}{2}2i\hbar\hat{x} = -\hat{x}\hat{y}^2 \tag{17}$$

Finally,

$$\boxed{\partial_t \hat{p}_x = -\hat{x}\hat{y}^2} \tag{18}$$

Likewise,

$$\boxed{\partial_t \hat{p}_y = -\hat{y}\hat{x}^2} \tag{19}$$

After obtained the Heisenberg equations, we can average the Eq. 13, 14, 18, 19 with the Wigner function in Eq. 3.

First, the following identity is essential to calculate an expectation value of an operator. It states that the expectation value of an operator can be obtained as a trace of the product of the density matrix and the operator.

$$\langle\hat{A}\rangle_\rho = \langle\psi|\hat{A}|\psi\rangle = Tr(\psi\rangle\langle\psi|\hat{A}) = Tr(\rho\hat{A}) \tag{20}$$

Therefore, let us average the first Heisenberg equation (Eq. 13) by using the trace function.

$$Tr(\rho\partial_t\hat{x}) = Tr(\rho\hat{p}_x) \tag{21}$$

$$\partial_t Tr(\rho\hat{x}) = Tr(\rho\hat{p}_x) \tag{22}$$

$$\partial_t\langle\hat{x}\rangle = \langle\hat{p}_x\rangle \tag{23}$$

$$\boxed{\partial_t x = p_x} \tag{24}$$

where $x \equiv \langle\hat{x}\rangle,\ y \equiv \langle\hat{y}\rangle,\ p_x \equiv \langle\hat{p}_x\rangle,\ p_y \equiv \langle\hat{p}_y\rangle$.

Likewise,

$$\boxed{\partial_t y = p_y} \tag{25}$$

For Eq. 18, the process is different from the previous part because of the products of coordinate and momentum operators, but still easy to track.

Remember, Eq. 18 is $\partial_t\hat{p}_x = -\hat{x}\hat{y}^2$. Then,

$$Tr(\rho\partial_t\hat{p}_x) = Tr(-\rho^2\hat{x}\hat{y}^2) \tag{26}$$

$$\partial_t p_x = -Tr(\rho^2\hat{x}\hat{y}^2) \tag{27}$$

$$= -\mathcal{N}^2 \int_{-\infty}^{\infty} d^4\xi\, e^{-\left(\xi-\bar{\xi}\right)\Sigma^{-1}\left(\xi-\bar{\xi}\right)} xy^2 \tag{28}$$

At this point, it is helpful to provide some gaussian integrals to clarify the further calculations.

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} x dx = 0 \tag{29}$$

$$\int_{-\infty}^{\infty} e^{-\alpha(x-x_0)^2} x dx \neq 0 \tag{30}$$

$$\int_{-\infty}^{\infty} e^{-\alpha(x-x_0)^2} (x - x_0 + x_0) dx \neq 0 \tag{31}$$

$$\int_{-\infty}^{\infty} e^{-\alpha(x-x_0)^2} (x - x_0) dx + \int_{-\infty}^{\infty} e^{-\alpha(x-x_0)^2} x_0 dx \neq 0 \tag{32}$$

$$\underbrace{\int_{-\infty}^{\infty} e^{-\alpha(x-x_0)^2}(x-x_0)dx}_{0} + \int_{-\infty}^{\infty} e^{-\alpha(x-x_0)^2} x_0 dx \neq 0 \tag{33}$$

Again, consider the integral

$$= -\mathcal{N}^2 \int_{-\infty}^{\infty} d^4\xi \, e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} xy^2 \tag{34}$$

Then use the technique mentioned above to manipulate the integral,

$$= -\mathcal{N}^2 \int_{-\infty}^{\infty} d^4\xi \, e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} (x-\overline{x}+\overline{x})(y-\overline{y}+\overline{y})^2 \tag{35}$$

$$= -\mathcal{N}^2 \int_{-\infty}^{\infty} d^4\xi \, ((x-\overline{x})+\overline{x})((y-\overline{y})+\overline{y})^2 e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} \tag{36}$$

$$= -\mathcal{N}^2 \int_{-\infty}^{\infty} d^4\xi \, \left((x-\overline{x})+\overline{x}\right)\left((y-\overline{y})^2 + 2\overline{y}(y-\overline{y}) + \overline{y}^2\right) e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} \tag{37}$$

$$= -\mathcal{N}^2 \left(\begin{array}{c} \int_{-\infty}^{\infty} d^4\xi \, (x-\overline{x})(y-\overline{y})^2 e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} + \\ \int_{-\infty}^{\infty} d^4\xi \, \left(2\overline{y}(x-\overline{x})(y-\overline{y}) + \overline{y}^2(x-\overline{x}) + \overline{x}(y-\overline{y})^2 + 2\overline{xy}(y-\overline{y}) + \overline{xy}^2\right) e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} \end{array} \right) \tag{38}$$

$$= -\left(\underbrace{\langle (x-\overline{x})(y-\overline{y})^2 \rangle}_{\#1} + \underbrace{2\overline{y}\langle (x-\overline{x})(y-\overline{y}) \rangle}_{\#2} + \underbrace{\overline{y}^2 \langle (x-\overline{x}) \rangle}_{\#3} + \underbrace{\overline{x}\langle (y-\overline{y})^2 \rangle}_{\#4} + \underbrace{2\overline{xy}\langle (y-\overline{y}) \rangle}_{\#5} + \overline{xy}^2 \right) \tag{39}$$

Notice that $\#1 = \langle (x-\overline{x})(y-\overline{y})^2 \rangle$ is zero because the integral is odd.

$$\mathcal{N}^2 \int_{-\infty}^{\infty} d^4\xi \, e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} (x-\overline{x})(y-\overline{y})^2 \tag{40}$$

To check this, let us show that the exponential term $e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)}$ is even under the transformation of $(x-\overline{x}) \rightarrow -(x-\overline{x})$. One needs to check the sign changes in Σ^{-1} too. For this, let us expand Σ further.

$$\Sigma_{ab} = \langle\langle \xi_a \xi_b \rangle\rangle \equiv \langle \frac{\hat{\xi}_a \hat{\xi}_b + \hat{\xi}_b \hat{\xi}_a}{2} \rangle - \langle \hat{\xi}_a \rangle \langle \hat{\xi}_b \rangle \tag{41}$$

$$\Sigma_{xx} = \langle \frac{\hat{x}\hat{x} + \hat{x}\hat{x}}{2} \rangle - \langle \hat{x} \rangle \langle \hat{x} \rangle = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 \tag{42}$$

$$\Sigma_{xy} = \langle \frac{\hat{x}\hat{y} + \hat{y}\hat{x}}{2} \rangle - \langle \hat{x} \rangle \langle \hat{y} \rangle = \langle \hat{x}\hat{y} \rangle - \langle \hat{x} \rangle \langle \hat{y} \rangle \tag{43}$$

$$\Sigma_{yx} = \langle \frac{\hat{y}\hat{x} + \hat{x}\hat{y}}{2} \rangle - \langle \hat{y} \rangle \langle \hat{x} \rangle = \langle \hat{x}\hat{y} \rangle - \langle \hat{x} \rangle \langle \hat{y} \rangle \tag{44}$$

$$\Sigma_{yy} = \langle \frac{\hat{y}\hat{y} + \hat{y}\hat{y}}{2} \rangle - \langle \hat{y} \rangle \langle \hat{y} \rangle = \langle \hat{y}^2 \rangle - \langle \hat{y} \rangle^2 \tag{45}$$

Let us take $\langle \hat{x} \rangle = \langle \hat{y} \rangle = 0$ for the sake of simplicity. Then,

$$\Sigma_{ab} = \begin{bmatrix} \langle \hat{x}^2 \rangle & \langle \hat{x}\hat{y} \rangle \\ \langle \hat{x}\hat{y} \rangle & \langle \hat{y}^2 \rangle \end{bmatrix} \tag{46}$$

$$\Sigma^{-1} = \frac{1}{\langle \hat{x}^2 \rangle \langle \hat{y}^2 \rangle - \langle \hat{x}\hat{y} \rangle^2} \begin{bmatrix} \langle \hat{y}^2 \rangle & -\langle \hat{x}\hat{y} \rangle \\ -\langle \hat{x}\hat{y} \rangle & \langle \hat{x}^2 \rangle \end{bmatrix} \tag{47}$$

Then the exponential term becomes

$$e^{-[x \quad y] \frac{1}{\langle \hat{x}^2 \rangle \langle \hat{y}^2 \rangle - \langle \hat{x}\hat{y} \rangle^2} \begin{bmatrix} \langle \hat{y}^2 \rangle & -\langle \hat{x}\hat{y} \rangle \\ -\langle \hat{x}\hat{y} \rangle & \langle \hat{x}^2 \rangle \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}} \tag{48}$$

$$e^{-\frac{1}{\langle \hat{x}^2 \rangle \langle \hat{y}^2 \rangle - \langle \hat{x}\hat{y} \rangle^2} \left(x^2 \langle \hat{y}^2 \rangle - 2xy \langle \hat{x}\hat{y} \rangle + y^2 \langle \hat{x}^2 \rangle \right)} \tag{49}$$

Finally,

$$\iint_{-\infty}^{\infty} dxdy e^{-\frac{1}{\langle \hat{x}^2 \rangle \langle \hat{y}^2 \rangle - \langle \hat{x}\hat{y} \rangle^2} \left(x^2 \langle \hat{y}^2 \rangle - 2xy \langle \hat{x}\hat{y} \rangle + y^2 \langle \hat{x}^2 \rangle \right)} xy^2 \tag{50}$$

as $x \to -x$, $xy^2 \to -xy^2$ and $\langle \hat{x}^2 \rangle \langle \hat{y}^2 \rangle - \langle \hat{x}\hat{y} \rangle^2 \to \langle \hat{x}^2 \rangle \langle \hat{y}^2 \rangle - \langle \hat{x}\hat{y} \rangle^2$, $x^2 \langle \hat{y}^2 \rangle \to x^2 \langle \hat{y}^2 \rangle$, $-2xy \langle \hat{x}\hat{y} \rangle \to -2 - xy \langle -\hat{x}\hat{y} \rangle = -2xy \langle \hat{x}\hat{y} \rangle$, $y^2 \langle \hat{x}^2 \rangle \to y^2 \langle \hat{x}^2 \rangle$. Therefore, the exponential term does not change sign. On the other hand, the rest, $(x - \overline{x})(y - \overline{y})^2$ is odd. Therefore, this integral is odd, and the value of the integral will be zero.

Furthermore, $\#3 = \overline{y}^2 \langle (x - \overline{x}) \rangle \; and \; \#5 = 2\overline{xy} \langle (y - \overline{y}) \rangle$ are zero because their integrals also will be odd.

We can expand $\#2 = 2\overline{y} \langle (x - \overline{x})(y - \overline{y}) \rangle$ by using the identity below.

$$\int_{-\infty}^{\infty} (x - \langle x \rangle)^2 |\psi|^2 dx \triangleq \langle x^2 \rangle - \langle x \rangle^2 \tag{51}$$

$$2\overline{y} \langle (x - \overline{x})(y - \overline{y}) \rangle = 2\overline{y} (\langle xy \rangle - \overline{xy}) \tag{52}$$

$$2\overline{y} \langle (x - \overline{x})(y - \overline{y}) \rangle = 2\overline{y} \langle xy \rangle - 2\overline{y}^2 \overline{x} \tag{53}$$

Likewise, for #4

$$\overline{x} \langle (y - \overline{y})^2 \rangle = \overline{x} \left(\langle y^2 \rangle - \overline{y}^2 \right) \tag{54}$$

$$\overline{x} \langle (y - \overline{y})^2 \rangle = \overline{x} \langle y^2 \rangle - \overline{xy}^2 \tag{55}$$

Then Eq. 39 becomes

$$= -\left(2\overline{y}\langle xy\rangle - 2\overline{y}^2\overline{x} + \overline{x}\langle y^2\rangle - \overline{xy}^2 + +\overline{xy}^2\right) \tag{56}$$

$$= -\left(2\overline{y}\langle xy\rangle - 2\overline{y}^2\overline{x} + \overline{x}\langle y^2\rangle\right) \tag{57}$$

$$= -\left(\overline{x}\langle y^2\rangle + 2\overline{y}\underbrace{\left(\langle xy\rangle - \overline{xy}\right)}_{\langle\langle xy\rangle\rangle}\right) \tag{58}$$

Then,

$$\partial_t p_x = -\overline{x}\langle y^2\rangle - 2\langle\langle xy\rangle\rangle\overline{y} \tag{59}$$

where $\bar{\xi}_a = \langle\hat{\xi}_a\rangle$, so

$$\partial_t p_x = -\langle\hat{x}\rangle\langle y^2\rangle - 2\langle\langle xy\rangle\rangle\langle\hat{y}\rangle \tag{60}$$

Finally,

$$\boxed{\partial_t p_x = -x\langle y^2\rangle - 2\langle\langle xy\rangle\rangle y} \tag{61}$$

Lastly, for Eq. 19

$$\partial_t \hat{p}_y = -\hat{y}\hat{x}^2 \tag{62}$$

$$Tr\left(\rho\partial_t\hat{p}_y\right) = Tr(-\rho^2\hat{y}\hat{x}^2) = -\langle\hat{y}\hat{x}^2\rangle \tag{63}$$

$$\partial_t p_y = -Tr(\rho^2\hat{x}\hat{y}^2) \tag{64}$$

$$= -\mathcal{N}^2\int_{-\infty}^{\infty} d^4\xi\, e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} yx^2 \tag{65}$$

$$= -\mathcal{N}^2\int_{-\infty}^{\infty} d^4\xi\left((y-\overline{y})+\overline{y}\right)\left((x-\overline{x})+\overline{x}\right)^2 e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} \tag{66}$$

$$= -\mathcal{N}^2\int_{-\infty}^{\infty} d^4\xi\left((y-\overline{y})+\overline{y}\right)\left((x-\overline{x})^2 + 2\overline{x}(x-\overline{x}) + \overline{x}^2\right) e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} \tag{67}$$

$$= -\mathcal{N}^2\left(\begin{array}{c}\displaystyle\int_{-\infty}^{\infty} d^4\xi\left((y-\overline{y})(x-\overline{x})^2\right)e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} + \\ \displaystyle\int_{-\infty}^{\infty} d^4\xi\left(2(y-\overline{y})(x-\overline{x})\overline{x} + (y-\overline{y})\overline{x}^2 + \overline{y}(x-\overline{x})^2 + 2\overline{y}(x-\overline{x})\overline{x} + \overline{yx}^2\right)e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)}\end{array}\right) \tag{68}$$

$$= -\left(\underbrace{\langle(y-\overline{y})(x-\overline{x})^2\rangle}_{=0} + 2\overline{x}\langle(y-\overline{y})(x-\overline{x})\rangle + \underbrace{\langle y-\overline{y}\rangle\overline{x}^2}_{=0} + \overline{y}\langle(x-\overline{x})^2\rangle + \underbrace{2\overline{y}\langle x-\overline{x}\rangle\overline{x}}_{=0} + \overline{yx}^2\right) \quad (69)$$

$$= -\left(2\overline{x}\underbrace{\langle(y-\overline{y})(x-\overline{x})\rangle}_{\langle yx\rangle-\overline{yx}} + \overline{y}\underbrace{\langle(x-\overline{x})^2\rangle}_{\langle x^2\rangle-\overline{x}^2} + \overline{yx}^2\right) \quad (70)$$

$$= -\left(2\overline{x}\langle yx\rangle - 2\overline{yx}^2 + \overline{y}\langle x^2\rangle - \overline{yx}^2 + \overline{yx}^2\right) \quad (71)$$

$$= -\left(\overline{y}\langle x^2\rangle + 2\overline{x}\underbrace{(\langle yx\rangle - \overline{yx})}_{\langle\langle yx\rangle\rangle}\right) \quad (72)$$

$$= -(\overline{y}\langle x^2\rangle + 2\langle\langle xy\rangle\rangle\overline{x}) \quad (73)$$

$$\partial_t p_y = -\overline{y}\langle x^2\rangle - 2\langle\langle xy\rangle\rangle\overline{x} \quad (74)$$

Finally,

$$\boxed{\partial_t p_y = -y\langle x^2\rangle - 2\langle\langle xy\rangle\rangle x} \quad (75)$$

Thus, 4 equations of motion (Equations 24, 25, 61, 75) were found for the Gaussian wave packet centers.

In the next step, to get equations for the dispersions $\langle\langle\xi_a\xi_b\rangle\rangle$, the Heisenberg equations of motion will be used one more time to obtain time derivative of the operator products $\hat{\xi}_a\hat{\xi}_b$,

$$\partial_t(\hat{x}\hat{x}) = \partial_t(\hat{x})\hat{x} + \hat{x}\partial_t(\hat{x}) \quad (76)$$

$$\partial_t(\hat{x}\hat{x}) = \hat{p}_x\hat{x} + \hat{x}\hat{p}_x \quad (77)$$

Similarly,

$$\partial_t(\hat{x}\hat{y}) = \hat{p}_x\hat{y} + \hat{x}\hat{p}_y \quad (78)$$

$$\partial_t(\hat{x}\hat{p}_x) = \hat{p}_x^2 - \hat{x}^2\hat{y}^2 \quad (79)$$

$$\partial_t(\hat{x}\hat{p}_y) = \hat{p}_x\hat{p}_y - \hat{x}^3\hat{y} \quad (80)$$

$$\partial_t(\hat{p}_x\hat{p}_x) = -\hat{x}\hat{y}^2\hat{p}_x - \hat{p}_x\hat{x}\hat{y}^2 \quad (81)$$

$$\partial_t(\hat{p}_x\hat{p}_y) = -\hat{x}\hat{y}^2\hat{p}_y - \hat{p}_x\hat{x}^2\hat{y} \quad (82)$$

Rest of the equations can be obtained by interchanging $x \leftrightarrow y$.

Again, same procedure can be repeated to get the equations of motion for Gaussian wave packet center.

As an example, for Equation (77),

$$Tr(\rho^2\partial_t\hat{x}\hat{x}) = Tr(\rho^2 2\hat{p}_x\hat{x}) = 2\langle\hat{p}_x\hat{x}\rangle \quad (83)$$

$$\partial_t\langle x^2\rangle = 2Tr(\rho^2\hat{p}_x\hat{x}) \quad (84)$$

$$= 2\mathcal{N}^2 \int_{-\infty}^{\infty} d^4\xi \, e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} x p_x \tag{85}$$

$$= 2\mathcal{N}^2 \int_{-\infty}^{\infty} d^4\xi \left((x-\overline{x})+\overline{x}\right)\left(\left(p_x-\overline{p}_x\right)+\overline{p}_x\right) e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} \tag{86}$$

$$= 2\mathcal{N}^2 \int_{-\infty}^{\infty} d^4\xi \left((x-\overline{x})\left(p_x-\overline{p}_x\right)+(x-\overline{x})\overline{p}_x+\overline{x}\left(p_x-\overline{p}_x\right)+\overline{xp}_x\right) e^{-\left(\xi-\overline{\xi}\right)\Sigma^{-1}\left(\xi-\overline{\xi}\right)} \tag{87}$$

$$= 2\left(\langle(x-\overline{x})\left(p_x-\overline{p}_x\right)\rangle+\underbrace{(x-\overline{x})\overline{p}_x}_{=0}+\underbrace{\overline{x}\left(p_x-\overline{p}_x\right)}_{=0}+\overline{xp}_x\right) \tag{88}$$

$$= 2\left(\underbrace{\langle(x-\overline{x})\left(p_x-\overline{p}_x\right)\rangle}_{\langle xp_x\rangle-\overline{xp}_x}+\overline{xp}_x\right) \tag{89}$$

$$= 2\left(\langle xp_x\rangle-\overline{xp}_x+\overline{xp}_x\right) \tag{90}$$

$$\partial_t\langle x^2\rangle = 2\langle xp_x\rangle \tag{91}$$

To find the equation of motion for the Gaussian wave packet dispersion, the following expression must be calculated.

$$\partial_t\langle\langle x^2\rangle\rangle = \partial_t\langle x^2\rangle - \partial_t\langle\hat{x}\rangle^2 \tag{92}$$

$$\partial_t\langle\langle x^2\rangle\rangle = \underbrace{\partial_t\langle x^2\rangle}_{=2\langle xp_x\rangle} - \underbrace{\partial_t\langle\hat{x}\rangle^2}_{=2\langle\hat{p}_x\rangle\langle\hat{x}\rangle} \tag{93}$$

Then,

$$\partial_t\langle\langle x^2\rangle\rangle = 2\langle xp_x\rangle - 2\langle\hat{p}_x\rangle\langle\hat{x}\rangle \tag{94}$$

$$\partial_t\langle\langle x^2\rangle\rangle = 2\left(\underbrace{\langle p_x x\rangle-\langle\hat{p}_x\rangle\langle\hat{x}\rangle}_{=\langle\langle p_x x\rangle\rangle}\right) \tag{95}$$

Finally,

$$\boxed{\partial_t\langle\langle x^2\rangle\rangle = 2\langle\langle p_x x\rangle\rangle} \tag{96}$$

The other equations of motion for the Gaussian wave packet dispersions can be found in the same way above.

$$\boxed{\partial_t\langle\langle y^2\rangle\rangle = 2\,\langle\langle p_y y\rangle\rangle} \tag{97}$$

$$\boxed{\partial_t\langle\langle xy\rangle\rangle = \langle\langle p_x y\rangle\rangle + \langle\langle x p_y\rangle\rangle} \tag{98}$$

$$\boxed{\partial_t\langle\langle x p_x\rangle\rangle = \langle\langle p_x p_x\rangle\rangle - \langle\langle x^2\rangle\rangle\langle y^2\rangle - 2\langle\langle xy\rangle\rangle\langle xy\rangle} \tag{99}$$

$$\boxed{\partial_t\,\langle\langle y p_y\rangle\rangle = \langle\langle p_y p_y\rangle\rangle - \langle\langle y^2\rangle\rangle\langle x^2\rangle - 2\langle\langle xy\rangle\rangle\langle xy\rangle} \tag{100}$$

$$\boxed{\partial_t\,\langle\langle x p_y\rangle\rangle = \langle\langle p_x p_y\rangle\rangle - \langle\langle xy\rangle\rangle\langle x^2\rangle - 2\langle\langle x^2\rangle\rangle\langle xy\rangle} \tag{101}$$

$$\boxed{\partial_t\langle\langle y p_x\rangle\rangle = \langle\langle p_x p_y\rangle\rangle - \langle\langle xy\rangle\rangle\langle y^2\rangle - 2\langle\langle y^2\rangle\rangle\langle xy\rangle} \tag{102}$$

$$\boxed{\partial_t\langle\langle p_x p_x\rangle\rangle = -2\langle\langle x p_x\rangle\rangle\langle y^2\rangle - 4\langle\langle y p_x\rangle\rangle\langle xy\rangle} \tag{103}$$

$$\boxed{\partial_t\,\langle\langle p_y p_y\rangle\rangle = -2\,\langle\langle y p_y\rangle\rangle\,\langle x^2\rangle - 4\,\langle\langle x p_y\rangle\rangle\,\langle xy\rangle} \tag{104}$$

$$\boxed{\partial_t\,\langle\langle p_x p_y\rangle\rangle = \langle\langle x p_y\rangle\rangle\,\langle y^2\rangle - 2\,\langle\langle y p_y\rangle\rangle\,\langle xy\rangle - \langle\langle y p_x\rangle\rangle\langle x^2\rangle - 2\langle\langle x p_x\rangle\rangle\langle xy\rangle} \tag{105}$$

Thus, instead of having 4 classical equations of motion, 14 equations of motion were obtained as a result of Gaussian state approximation.

3) Results and Discussion

After obtaining the complete system of equations, those 14 equations of motion were solved in MATLAB numerically by using the ode45 function and handwritten 4th order Runge-Kutta method. The codes can be found in the Appendices section.

To solve the complete system of equations, the following initial conditions were used to keep the quantum dispersions minimal.

$$x = 0.625f, \quad y = 0.325f, \quad \langle\langle xx \rangle\rangle = \langle\langle yy \rangle\rangle = \langle\langle p_x p_x \rangle\rangle = \langle\langle p_y p_y \rangle\rangle = 0.5 \tag{106}$$

$$p_x = p_y = \langle\langle xy \rangle\rangle = \langle\langle p_x p_y \rangle\rangle = \langle\langle p_x x \rangle\rangle = \langle\langle p_x y \rangle\rangle = \langle\langle p_y x \rangle\rangle = \langle\langle p_y y \rangle\rangle = 0 \tag{107}$$

The variable f emphasizes the weight of the classical expectation values $\langle x \rangle$ and $\langle y \rangle$ over the quantum dispersions. In this way, the behaviour of the system was inspected by changing the expectation values of x and y.

The time evolution of the system for certain values of f can be seen in the figures below.

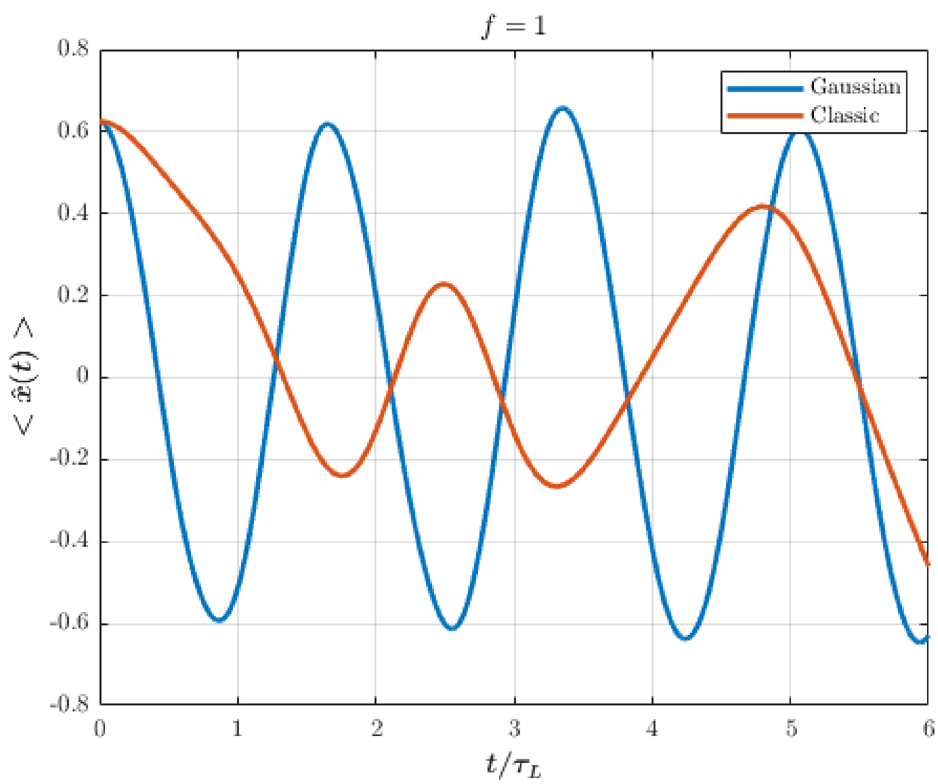

Figure 1 The time dependence of $x \equiv \langle \hat{x}(t) \rangle$ when $f = 1$.

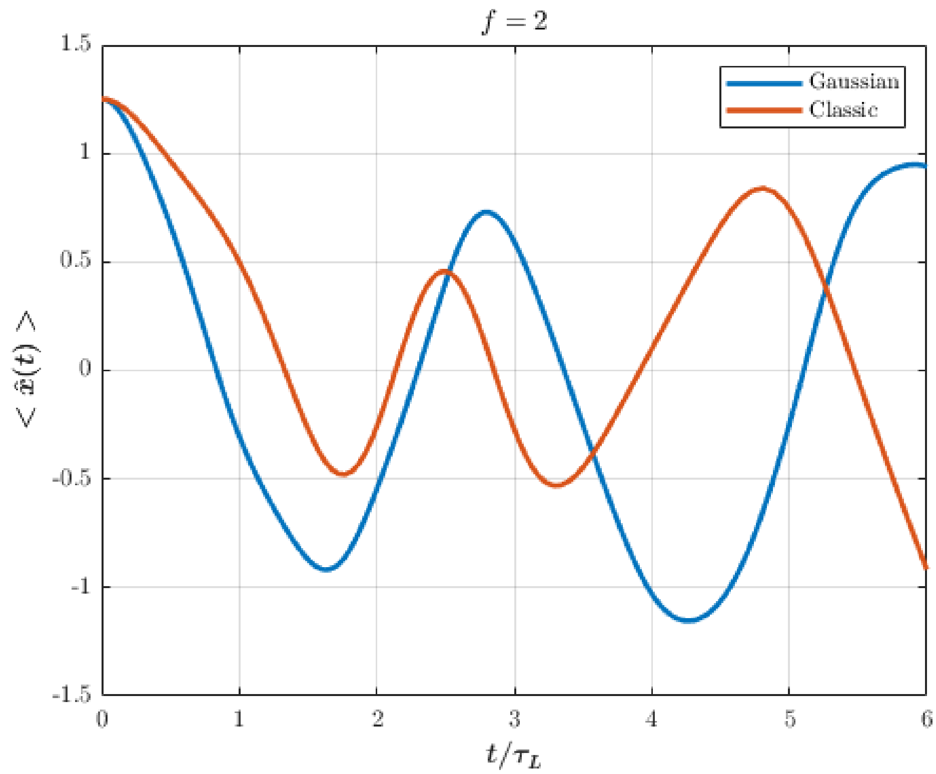

Figure 2 The time dependence of $x \equiv \langle \hat{x}(t) \rangle$ *when* $f = 2$.

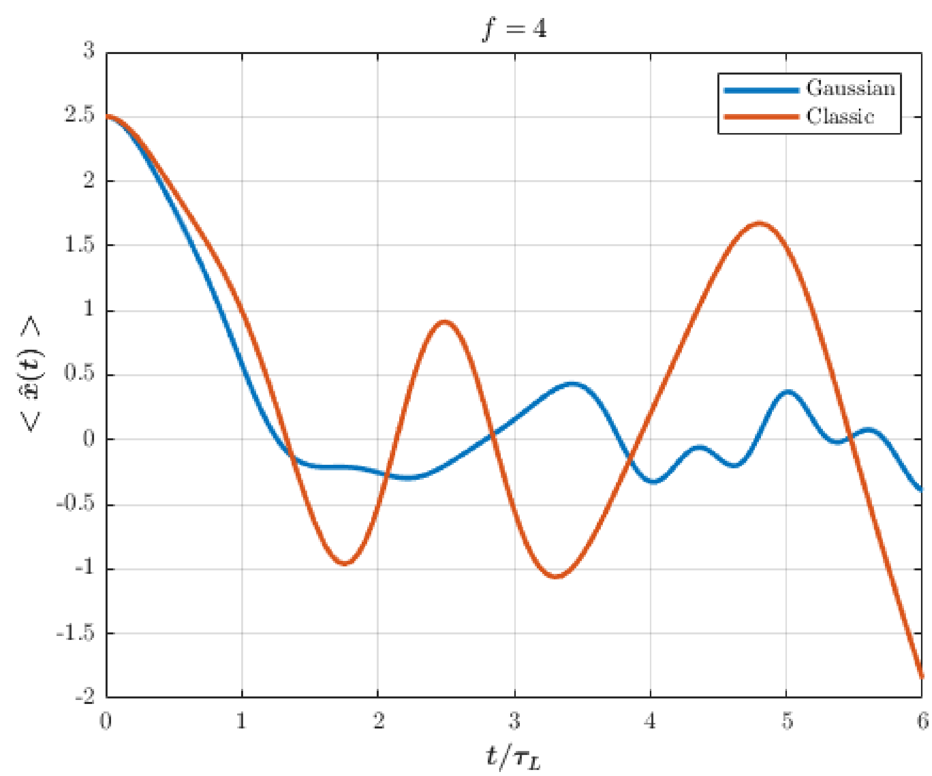

Figure 3 The time dependence of $x \equiv \langle \hat{x}(t) \rangle$ *when* $f = 4$.

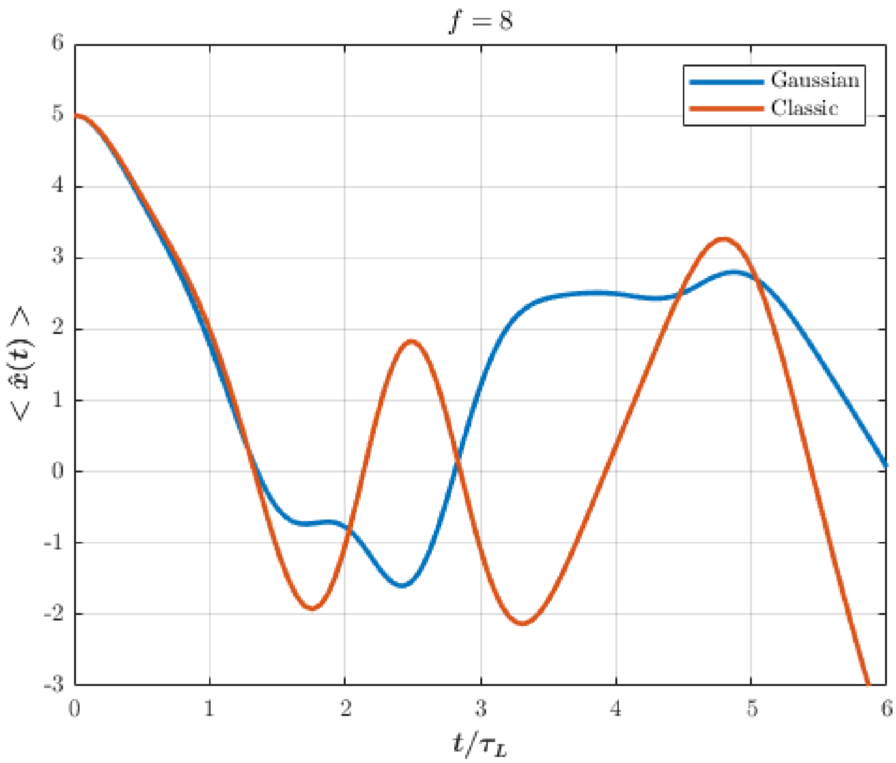

Figure 4 The time dependence of $x \equiv \langle \hat{x}(t) \rangle$ when $f = 8$.

For different values of f, the time evolutions of the expectation value of $\hat{x}$ operator i.e., the center of a Gaussian wave packet, were analyzed. As f increases, the behaviour of the system moves from the quantum regime to the classical regime as expected. At the large f values, these regimes match for early times.

For this PHYS400 project, our aim was to compare the solutions of classical and Gaussian state equations of motions with the exact solution of the time-dependent Schrödinger equation. We expect that for the small values of f, the solution of the Gaussian state approximation will be more convenient than the solution of classical equations of motion when compared to the time evolution of the Schrödinger equation because the Gaussian state approximation takes into account the quantum effects of the wave function of the system. However, I could not solve the 2D time-dependent Schrödinger equation yet. When I solve that equation, the graphs in Figure 1 will make more sense.

4) Conclusion

In conclusion, the importance of a quantum mechanical approximation for the classically chaotic systems has been observed because classical equations of motion lack the quantum effects which lead not to study current physics problems. During my project, I have learned how to approach a theoretical physics problem and solve that problem numerically using a programming language. Many thanks to my dear Professor Seçkin Kürkçüoğlu for his patience, guidance, and effort since the beginning of the term.

As future work, I am planning to solve the 2D Schrödinger equation numerically and compare the results with the plots in Figure 1. For this purpose, I am planning to use the split step Fourier transform [11-14] and the finite difference time domain (FDTD) method [15-17]. These methods are very common in the scientific environment and I want to experience how to solve a Schrödinger equation numerically because solving a time-dependent Schrödinger equation exactly is not that easy. Therefore, I am accepting this challenge as an opportunity to go beyond my previous skills.

5) References

[1] Buividovich P., Hanada M., Schäfer A., EPJ Web Conf.175, 08006 (2018) [arXiv:1711.05556 [hep-th]]

[2] Balasubramanian V., et al., Phys. Rev. Lett. 106, 191601 (2011), ArXiv:1012.4753

[3] Kurkela A., Moore G. D., JHEP 1112, 044 (2011), ArXiv:1107.5050

[4] Pratt S., et al., Phys. Rev. Lett. 111, 222302 (2013), ArXiv:1307.2539

[5] Chesler P. M., Yaffe L. G., JHEP 1407, 086 (2014), ArXiv:1309.1439

[6] Dusling K., Epelbaum T., Gelis F., Venugopalan R., Nucl. Phys. A 850, 69 (2011), ArXiv:1009.4363

[7] Kunihiro T., Müller B., Ohnishi A., Schäfer A., Prog. Theor. Phys. 121, 555 (2009), ArXiv:0809.4831

[8] Arnold P., Moore G.D., Yaffe L.G., JHEP 0301, 030 (2003), ArXiv:hep-ph/0209353

[9] Kurkela A., Zhu Y., Phys. Rev. Lett. 115, 182301 (2015), ArXiv:1506.06647

[10] Savvidy G. K., Nucl. Phys. B 246, 302 (1984)

[11] The Split-Operator Method. Retrieved from https://www.algorithm-archive.org/contents/split-operator_method/split-operator_method.html

[12] Time Evolution Split Operator Method. Retrieved from http://albi3ro.github.io/M4/Time-Evolution.html

[13] Time Evolution in Quantum Mechanics. Retrieved from https://ocw.mit.edu/courses/nuclear-engineering/22-02-introduction-to-applied-nuclear-physics-spring-2012/lecture-notes/MIT22_02S12_lec_ch6.pdf

[14] Split Step Fourier Method. Retrieved from https://www.mathworks.com/matlabcentral/fileexchange/14915-split-step-fourier-method

[15] On the stability of the FDTD method for solving a time-dependent Schrödinger equation. Retrieved from https://onlinelibrary.wiley.com/doi/epdf/10.1002/num.20082

[16] A G-FDTD Method for Solving the Multi-Dimensional Time-Dependent Schrödinger Equation. Retrieved from https://arxiv.org/ftp/arxiv/papers/1212/1212.0801.pdf

[17] Solving the Schrödinger equation using the finite difference time domain method. Retrieved from https://www.astrosen.unam.mx/~aceves/Fisica_Computacional/ebooks/fdtd-QM-Sudiarta2007.pdf

6) Appendices

6.1) ode45 Codes

```
% Rafet KAVAK - 2166783
% PHYS400 Project - 22.06.2021
% v2 - 12.07.2021

clc; % Clears the Command Window
close all; % Closes the all figures
clear; % Clears the Workspace

set(groot,'defaulttextinterpreter','latex');
set(groot, 'defaultAxesTickLabelInterpreter','latex');
set(groot, 'defaultLegendInterpreter','latex');

%{
Variables
------------------------------
    x      ------> x1
    y      ------> x2
   p_x     ------> x3
   p_y     ------> x4
 <<x^2>>   ------> x5
 <<y^2>>   ------> x6
  <<xy>>   ------> x7
 <<xp_x>>  ------> x8
 <<yp_y>>  ------> x9
 <<xp_y>>  ------> x10
 <<yp_x>>  ------> x11
<<p_xp_x>> ------> x12
<<p_yp_y>> ------> x13
<<p_xp_y>> ------> x14



Variable Matrix
------------------------------
x = [x1;  = x(1)
     x2;  = x(2)
     x3;  = x(3)
     x4;  = x(4)
     x5;  = x(5)
     x6;  = x(6)
     x7;  = x(7)
     x8;  = x(8)
     x9;  = x(9)
     x10;  = x(10)
     x11;  = x(11)
     x12;  = x(12)
     x13;  = x(13)
     x14]  = x(14)
```

```
Initial Conditions
-----------------------------
x0 = [0.625*factor;  = x1(0)
      0.325*factor;  = x2(0)
        0;           = x3(0)
        0;           = x4(0)
       0.5;          = x5(0)
       0.5;          = x6(0)
        0;           = x7(0)
        0;           = x8(0)
        0;           = x9(0)
        0;           = x10(0)
        0;           = x11(0)
       0.5;          = x12(0)
       0.5;          = x13(0)
        0];          = x14(0)
%}

%
tStart = tic;

% f and Initial Conditions
f  =
@(t,x)([f1(t,x);f2(t,x);f3(t,x);f4(t,x);f5(t,x);f6(t,x);f7(t,x);f8(t,x);f9(t,x);f10(t,x);f11(t,x)
;f12(t,x);f13(t,x);f14(t,x)]);

f_classical = @(t2,x2)([fc1(t2,x2);fc2(t2,x2);fc3(t2,x2);fc4(t2,x2)]);

factor = 8;

x0 = [0.625*factor;
      0.325*factor;
        0;
        0;
       0.5;
       0.5;
        0;
        0;
        0;
        0;
        0;
       0.5;
       0.5;
        0];

xc0 = [0.625*factor;
      0.325*factor;
        0;
        0];

% ode45
tspan = [0 3.75];
```

```
[t,x] = ode45(@appr, tspan, x0);
[t2,x2] = ode45(@appr2, tspan, xc0);


close all; % Closes the all figures
figure;
%for f = 1: tspan = [0 30] and plot(t/15*3...
%for f = 2: tspan = [0 15] and plot(t/15*6...
%for f = 4: tspan = [0 7.5] and plot(t/15*12...
%for f = 8: tspan = [0 3.75] and plot(t/15*24...
plot(t/15*24,x(:,1),'LineWidth',2), grid;
xlabel('{\boldmath$t/\tau_{L}$}'), ylabel('{\boldmath$<\hat{x}(t)>$}');
factorstr = sprintf('$f = %.0f$', factor);

title(factorstr);
%for f = 1: ylim([-0.8 0.8]);
%for f = 2: ylim([-1.5 1.5]);
%for f = 4: ylim([-2 3]);
%for f = 8: ylim([-3 6]);
ylim([-3 6]);
hold on

%for f = 1: tspan = [0 30] and plot(t/15*3...
%for f = 2: tspan = [0 15] and plot(t/15*6...
%for f = 4: tspan = [0 7.5] and plot(t/15*12...
%for f = 8: tspan = [0 3.75] and plot(t/15*24...
plot(t2/15*24,x2(:,1),'LineWidth',2), grid on;

legend('Gaussian', 'Classic');

% set(gca,'LooseInset',get(gca,'TightInset'));
% saveas(gcf,'junk.eps')
%
% set(findall(gcf,'Type','line'),'LineWidth',2)
% set(findall(gcf,'-property','FontSize'),'FontSize',12);

tEnd = toc(tStart)

function dxdt = appr(t,x)

dxdt = [x(3);
        x(4);
        -x(1)*(x(6)+x(2)^2)-2*x(7)*x(2);
        -x(2)*(x(5)+x(1)^2)-2*x(7)*x(1);
        2*x(8);
        2*x(9);
        x(11)+x(10);
        x(12)-x(5)*(x(6)+x(2)^2)-2*x(7)*(x(7)+x(1)*x(2));
        x(13)-x(6)*(x(5)+x(1)^2)-2*x(7)*(x(7)+x(1)*x(2));
        x(14)-x(7)*(x(5)+x(1)^2)-2*x(5)*(x(7)+x(1)*x(2));
        x(14)-x(7)*(x(6)+x(2)^2)-2*x(6)*(x(7)+x(1)*x(2));
        -2*x(8)*(x(6)+x(2)^2)-4*x(11)*(x(7)+x(1)*x(2));
        -2*x(9)*(x(5)+x(1)^2)-4*x(10)*(x(7)+x(1)*x(2));
        -x(10)*(x(6)+x(2)^2)-2*x(9)*(x(7)+x(1)*x(2))-x(11)*(x(5)+x(1)^2)-
```

```
2*x(8)*(x(7)+x(1)*x(2))];
end
function dxdt2 = appr2(t2,x2)

dxdt2 = [x2(3);
        x2(4);
        -x2(1)*(x2(2)^2);
        -x2(2)*(x2(1)^2)];
end
```

Published with MATLAB® R2020b

6.2) RK4 Codes

```
% Rafet KAVAK - 2166783
% PHYS400 Project - 22.06.2021
% v2 - 12.07.2021

clc; % Clears the Command Window
close all; % Closes the all figures
clear; % Clears the Workspace

set(groot,'defaulttextinterpreter','latex');
set(groot, 'defaultAxesTickLabelInterpreter','latex');
set(groot, 'defaultLegendInterpreter','latex');

%
tStart = tic;

% f and Initial Conditions
f1 = @(t,x)(x(3));
f2 = @(t,x)(x(4));
f3 = @(t,x)(-x(1)*(x(6)+x(2)^2)-2*x(7)*x(2));
f4 = @(t,x)(-x(2)*(x(5)+x(1)^2)-2*x(7)*x(1));
f5 = @(t,x)(2*x(8));
f6 = @(t,x)(2*x(9));
f7 = @(t,x)(x(11)+x(10));
f8 = @(t,x)(x(12)-x(5)*(x(6)+x(2)^2)-2*x(7)*(x(7)+x(1)*x(2)));
f9 = @(t,x)(x(13)-x(6)*(x(5)+x(1)^2)-2*x(7)*(x(7)+x(1)*x(2)));
f10 = @(t,x)(x(14)-x(7)*(x(5)+x(1)^2)-2*x(5)*(x(7)+x(1)*x(2)));
f11 = @(t,x)(x(14)-x(7)*(x(6)+x(2)^2)-2*x(6)*(x(7)+x(1)*x(2)));
f12 = @(t,x)(-2*x(8)*(x(6)+x(2)^2)-4*x(11)*(x(7)+x(1)*x(2)));
f13 = @(t,x)(-2*x(9)*(x(5)+x(1)^2)-4*x(10)*(x(7)+x(1)*x(2)));
f14 = @(t,x)(-x(10)*(x(6)+x(2)^2)-2*x(9)*(x(7)+x(1)*x(2))-x(11)*(x(5)+x(1)^2)-
2*x(8)*(x(7)+x(1)*x(2)));

f  =
@(t,x)([f1(t,x);f2(t,x);f3(t,x);f4(t,x);f5(t,x);f6(t,x);f7(t,x);f8(t,x);f9(t,x);f10(t,x);f11(t,x)
;f12(t,x);f13(t,x);f14(t,x)]);

factor = 4;

x0 = [0.625*factor; %x1
```

```
      0.325*factor;
        0;
        0;
       0.5;
       0.5;
        0;
        0;
        0;
        0;
        0;
       0.5;
       0.5;
        0];


% Sim Parameters
tend  = 6;
h     = 0.001;      % initial step size

% Simulation
clear x time;
x(:,1) = x0;                % state values during the simulation
time(1) = 0;                % simulation time

for kk = 1:tend/h
    x(:,kk+1) = RKmP4(time(kk),x(:,kk),h,f);
    time(kk+1) = kk*h;
end

figure;
plot(time,x(1,:),'LineWidth',2), grid;
xlabel('{\boldmath$t/\tau_{L}$}'), ylabel('{\boldmath$<\hat{x}(t)>$}');
factorstr = sprintf('$f = %.0f$', factor);
legend(factorstr);
title('$dx/dt = f(x)$');

%for f = 1: ylim([-0.8 0.8]);
%for f = 2: ylim([-1.5 1.5]);
%for f = 4: ylim([-2 3]);
%for f = 8: ylim([-3 6]);
ylim([-3 6]);

tEnd = toc(tStart)

function xNext = RKmP4(t,x,h,f)
c2 = 1/2;
c3 = 1/2;
c4 = 1;
b1 = 1/6;
b2 = 2/6;
b3 = 2/6;
b4 = 1/6;
a21 = 1/2;
a31 = 0;
```

```
a32 = 1/2;
a41 = 0;
a42 = 0;
a43 = 1;

k1 = f(t, x);
k2 = f(t+c2*h, x+h*a21*k1);
k3 = f(t+c3*h, x+h*a31*k1+h*a32*k2);
k4 = f(t+c4*h, x+h*a41*k1+h*a42*k2+h*a43*k3);
xNext = x+h*(b1*k1+b2*k2+b3*k3+b4*k4);
end
```

Published with MATLAB® R2020b