# A new real-time technique to study chaotic dynamics at quantum level

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- Blends analytical quantum mechanical concepts and numerical techniques



#### Aim

Proposing a quantum mechanical approximation, (Gaussian state approximation), to a classically chaotic system and investigating its time evolution

These kind of chaotic systems can be represented by the Hamiltonian (1)

$$H = \frac{1}{2} \sum_{i} \operatorname{Tr} P_{i}^{2} - \frac{1}{4} \sum_{i,j} \operatorname{Tr} [X_{i}, X_{j}]^{2}$$
 (1)

The distance between initially very close points grows exponentially with time

Such chaotic systems forget about initial conditions after some time

#### Remark

Hamiltonian (1) can give some insight into the formation of Black holes[2]

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#### Method

The simplest example of the Hamiltonian (1)

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

- For a given Hamiltonian (2), we will find the Heisenberg equations at first
- Then we will find the equations of motion by taking averages of the Heisenberg equations



### Heisenberg Equations

#### Heisenberg Equation

$$\frac{d}{dt}A_{H}(t) = \frac{i}{\hbar}\left[H_{H}, A_{H}(t)\right] + \left(\frac{\partial A_{S}}{\partial t}\right)_{H}$$
(3)

where  $H_H$  is Hamiltonian operator and  $A_H(t)$  is a canonically conjugate operator.



### Derivation of the 1<sup>st</sup> Heisenberg Equation

$$\frac{d\hat{x}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{x}] + \frac{\partial \hat{x}}{\partial t} \tag{4}$$

$$\frac{d\hat{x}}{dt} = \frac{i}{\hbar} \left[ \frac{\hat{p}_x^2}{2} + \frac{\hat{p}_y^2}{2} + \frac{\hat{x}^2 \hat{y}^2}{2}, \hat{x} \right] + \frac{\partial \hat{x}}{\partial t}$$
 (5)

$$\frac{d\hat{x}}{dt} = \frac{i}{\hbar} \left[ \frac{\hat{p}_x^2}{2}, \hat{x} \right] = \frac{i}{\hbar} \left( \frac{\hat{p}_x}{2} \left[ \hat{p}_x, \hat{x} \right] + \left[ \hat{p}_x, \hat{x} \right] \frac{\hat{p}_x}{2} \right) \tag{6}$$

$$\frac{d\hat{x}}{dt} = \frac{i}{\hbar}\hat{p}_{x}\left[\hat{p}_{x},\hat{x}\right] \quad \text{where} \quad \left[\hat{x},\hat{p}_{x}\right] = i\hbar \tag{7}$$

$$d_t \hat{x} = \hat{p}_x \tag{8}$$



### Heisenberg Equations

Heisenberg equations for canonically conjugate operators  $\hat{x}$ ,  $\hat{y}$ ,  $\hat{p}_x$ ,  $\hat{p}_y$ 

$$d_t \hat{x} = \hat{p}_x \tag{9}$$

$$d_t \hat{y} = \hat{\rho}_y \tag{10}$$

$$d_t \hat{\rho}_{\mathsf{x}} = -\hat{x}\hat{y}^2 \tag{11}$$

$$d_t \hat{p}_y = -\hat{y}\hat{x}^2 \tag{12}$$



### Finding Equations of Motion

Let us find the equation of motion for the first Heisenberg equation  $d_t \hat{x} = \hat{p}_x$ .

We can take the average of the Heisenberg equation by using the following theorem.

#### Trace Function to Calculate Expectation Values

The expectation value of an operator can be found by

$$\langle \psi | \hat{A} | \psi \rangle = \langle \hat{A} \rangle_{\rho} = \text{Tr} \left( \rho \hat{A} \right)$$
 (13)

where  $\rho$  is the density matrix.



# Example for the 1<sup>st</sup> Heisenberg Equation

Then by averaging the  $1^{st}$  Heisenberg equation  $d_t \hat{x} = \hat{p}_x$ ,

$$\langle d_t \hat{x} \rangle = \langle \hat{p}_x \rangle \tag{14}$$

$$\operatorname{Tr}\left(\rho d_{t}\hat{x}\right) = \operatorname{Tr}\left(\rho \hat{p}_{x}\right) \tag{15}$$

$$d_t \operatorname{Tr}(\rho \hat{x}) = \operatorname{Tr}(\rho \hat{p}_x) \tag{16}$$

$$d_t \langle \hat{x} \rangle = \langle \hat{p}_x \rangle \tag{17}$$

$$d_t x = p_x \tag{18}$$

where

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

# Example for the 3<sup>rd</sup> Heisenberg Equation

Remember,  $3^{rd}$  Heisenberg Equation is  $d_t \hat{p}_x = -\hat{x}\hat{y}^2$ . Then,

$$\operatorname{Tr}\left(\rho d_{t}\hat{p}_{x}\right) = -\operatorname{Tr}\left(\rho\hat{x}\hat{y}^{2}\right) \tag{19}$$

$$d_t \operatorname{Tr}(\rho \hat{p}_x) = -\operatorname{Tr}(\rho \hat{x} \hat{y}^2)$$
 (20)

$$d_t \langle \hat{p}_x \rangle = -\int_{-\infty}^{\infty} d^n(x, y) \, \rho x y^2 \tag{21}$$

The upper integral yields another expectation values and the more number of expectation values of coordinate/momentum operators involve. We need an approximation to truncate these infinite set of equations!



### The Gaussian State Approximation

Solution: Characterizing the density matrix  $\rho$  by the Gaussian state Wigner function. Thus, we could express the expectation values of products of coordinate/momentum operators in terms of Gaussian wave packet centers and Gaussian wave packet dispersions

$$\rho(\xi) = \mathcal{N}\exp\left(-\frac{1}{2}(\xi - \bar{\xi})\Sigma^{-1}(\xi - \bar{\xi})\right)$$
 (22)

$$\bar{\xi}_{\mathsf{a}} \equiv \langle \hat{\xi}_{\mathsf{a}} \rangle \tag{23}$$

$$\Sigma_{ab} = \langle \langle \xi_a \xi_b \rangle \rangle \equiv \langle \frac{\hat{\xi}_a \hat{\xi}_b + \hat{\xi}_b \hat{\xi}_a}{2} \rangle - \langle \hat{\xi}_a \rangle \langle \hat{\xi}_b \rangle$$
 (24)

where  $\xi = \{x, y, p_x, p_y\}$  is the vector which consists of classical phase space variables.  $\bar{\xi}_a \equiv \langle \hat{\xi}_a \rangle$  indicates the Gaussian wave packet centers and  $\langle \langle \xi_a \xi_b \rangle \rangle$  indicates the Gaussian wave packet dispersions

### Again for 3rd Heisenberg Equation

$$\operatorname{Tr}\left(\rho d_{t}\hat{p}_{x}\right) = -\operatorname{Tr}\left(\rho\hat{x}\hat{y}^{2}\right) \tag{25}$$

$$d_t \langle \hat{p}_x \rangle = \int_{-\infty}^{\infty} d^4(\xi) \, \rho(\xi) x y^2 \tag{26}$$

$$d_t \langle \hat{p}_x \rangle = -\mathcal{N}^2 \int_{-\infty}^{\infty} d^4(\xi) \, e^{-(\xi - \bar{\xi})\Sigma^{-1}(\xi - \bar{\xi})} x y^2 \tag{27}$$

After long calculations

$$d_t p_x = -x \langle y^2 \rangle - 2 \langle \langle xy \rangle \rangle y, \tag{28}$$

In this way, 4 equations of motion for the Gaussian wave packet centers and 10 equations of motion for Gaussian wave packet dispersions were found.

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## Complete System of Equations

```
1^{st}: \partial_t \langle \hat{x} \rangle = p_x
2^{nd}: \partial_t \langle \hat{y} \rangle = p_V
3^{rd}: \partial_t \langle \hat{p}_x \rangle = -x \langle y^2 \rangle - 2 \langle \langle xy \rangle \rangle y
4^{th}: \partial_t \langle \hat{p}_v \rangle = -y \langle x^2 \rangle - 2 \langle \langle xy \rangle \rangle x
5^{th}: \partial_t \langle \langle x^2 \rangle \rangle = 2 \langle \langle p_x x \rangle \rangle
6^{th}: \partial_t \langle \langle y^2 \rangle \rangle = 2 \langle \langle p_y y \rangle \rangle
7^{th} : \partial_t \langle \langle xy \rangle \rangle = \langle \langle p_x y \rangle \rangle + \langle \langle x p_y \rangle \rangle
8^{th}: \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 x y \rangle \rangle \langle x y \rangle
9^{th}: \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
10^{th}: \partial_t \langle \langle x p_v \rangle \rangle = \langle \langle p_x p_v \rangle \rangle - \langle \langle x y \rangle \rangle \langle x^2 \rangle - 2 \langle \langle x^2 \rangle \rangle \langle x y \rangle
11^{th}: \partial_t \langle \langle y p_x \rangle \rangle = \langle \langle p_x p_y \rangle \rangle - \langle \langle x y \rangle \rangle \langle y^2 \rangle - 2 \langle \langle y^2 \rangle \rangle \langle x y \rangle
12^{th}: \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 x y \rangle
13^{th}: \partial_t \langle \langle p_v p_v \rangle \rangle = -2 \langle \langle y p_v \rangle \rangle \langle x^2 \rangle - 4 \langle \langle x p_v \rangle \rangle \langle x y \rangle
14^{th}: \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 x y \rangle - \langle \langle y p_x \rangle \rangle \langle x^2 \rangle - 2 \langle \langle x p_x \rangle \rangle \langle x y \rangle
 (29)
```

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5^{th}: \partial_t \langle \langle x^2 \rangle \rangle = 2 \langle \langle p_x x \rangle \rangle
6^{th}: \partial_t \langle \langle v^2 \rangle \rangle = 2 \langle \langle p_v y \rangle \rangle
7^{th} : \partial_t \langle \langle xy \rangle \rangle = \langle \langle p_x y \rangle \rangle + \langle \langle x p_y \rangle \rangle
8^{th}: \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 x y \rangle \rangle \langle x y \rangle
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(30)
```

#### Initial conditions

Quantum dispersions were kept minimal

$$x = 0.625f, \quad y = 0.325f, \quad \langle\langle x^2 \rangle\rangle = \langle\langle y^2 \rangle\rangle = \langle\langle p_x^2 \rangle\rangle = \langle\langle p_y^2 \rangle\rangle = \frac{1}{2},$$

$$p_x = p_y = \langle\langle xy \rangle\rangle = \langle\langle p_x p_y \rangle\rangle = \langle\langle p_x x \rangle\rangle = \langle\langle p_x y \rangle\rangle = \langle\langle p_y y \rangle\rangle = 0$$
(31)



```
1^{st}:\langle \hat{x}\rangle \longrightarrow x_1
2^{nd}:\langle \hat{y}\rangle \longrightarrow x_2
3^{rd}:\langle \hat{p}_x\rangle \longrightarrow x_3
4^{th}:\langle \hat{p}_{v}\rangle \longrightarrow x_{4}
5^{th}: \langle \langle x^2 \rangle \rangle \longrightarrow x_5
6^{th}: \langle \langle v^2 \rangle \rangle \longrightarrow x_6
7^{th}: \langle \langle xy \rangle \rangle \longrightarrow x_7
8^{th}:\langle\langle xp_x\rangle\rangle\longrightarrow x_8
9^{th}:\langle\langle yp_v\rangle\rangle\longrightarrow x_9
10^{th}:\langle\langle xp_{\nu}\rangle\rangle\longrightarrow x_{10}
11^{th}: \langle \langle vp_x \rangle \rangle \longrightarrow x_{11}
12^{th}:\langle\langle p_x p_x\rangle\rangle\longrightarrow x_{12}
13^{th}: \langle\langle p_{\nu}p_{\nu}\rangle\rangle \longrightarrow x_{13}
14^{th}:\langle\langle p_{x}p_{y}\rangle\rangle\longrightarrow x_{14}
(32)
```

$$1^{st} : \partial_t x_1 = x_3 
2^{nd} : \partial_t x_2 = x_4 
3^{rd} : \partial_t x_3 = -x_1(x_6 + x_2^2) - 2x_7x_2 
4^{th} : \partial_t x_4 = -x_2(x_5 + x_2^2) - 2x_7x_1 
5^{th} : \partial_t x_5 = 2x_8 
6^{th} : \partial_t x_7 = x_{11} + x_{10} 
8^{th} : \partial_t x_8 = x_{12} - x_5(x_6 + x_2^2) - 2x_7(x_7 + x_1x_2) 
9^{th} : \partial_t x_9 = x_{13} - x_6(x_5 + x_1^2) - 2x_7(x_7 + x_1x_2) 
10^{th} : \partial_t x_{10} = x_{14} - x_7(x_5 + x_1^2) - 2x_5(x_7 + x_1x_2) 
11^{th} : \partial_t x_{11} = x_{14} - x_7(x_6 + x_2^2) - 2x_6(x_7 + x_1x_2) 
12^{th} : \partial_t x_{12} = -2x_8(x_6 + x_2^2) - 4x_{11}(x_7 + x_1x_2) 
13^{th} : \partial_t x_{13} = -2x_9(x_5 + x_1^2) - 4x_{10}(x_7 + x_1x_2) 
14^{th} : \partial_t x_{14} = -x_{10}(x_6 + x_2^2) - 2x_9(x_7 + x_1x_2) - x_{11}(x_5 + x_1^2) - 2x_8(x_7 + x_1x_2) 
(33)$$

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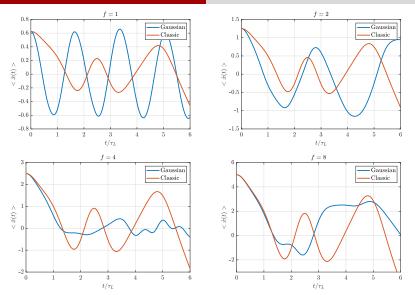


Figure 1: The comparison of the time dependence of  $\bar{x} \equiv \langle \hat{x}(t) \rangle$ , the center of a Gaussian wave packet, according to certain f values

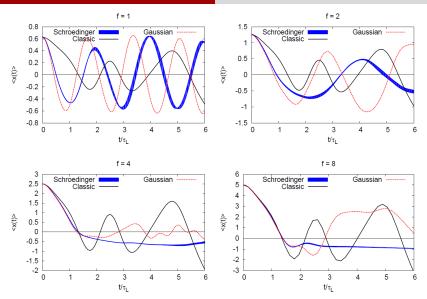


Figure 2: Article's plots with the exact solution of Schrödinger equation

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- I have learned how to approach a theoretical physics problem and solve that problem numerically using a programming language.
- Many thanks to my supervisor Prof. Seçkin Kürkçüoğlu for his patience, guidance and effort.
- As future work, I am planning to solve the 2D Schrödinger equation numerically and compare the results with the plots in Figure 1.



# Thank you!

Thank you very much for your interest and attention.



### Questions?

Any Questions?



### References



Pavel Buividovich, Masanori Hanada, and Andreas Schäfer. "Real-time dynamics of matrix quantum mechanics beyond the classical approximation". In: *EPJ Web of Conferences* 175 (2018). Ed. by M. Della Morte et al., p. 08006. ISSN: 2100-014X. DOI: 10.1051/epjconf/201817508006. URL: http://dx.doi.org/10.1051/epjconf/201817508006.