# Métodos computacionais em física
# Project 4 - Report

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## 1 Introduction

This project had as objective a numerical simulation of a unidimensional quantum harmonic oscillator. Given initial conditions we want to determine the solution of the Schrodinger equation:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \tag{1}$$

$\hbar$ is the reduced planck constant, $m$ is the mass, $i$ is the complex unit and $V(x)$ is the potential of a harmonic oscillator:

$$V(x) = \frac{m}{2}\omega^2 x^2 \tag{2}$$

Where $\omega$ is the angular frequency. The time independent Schrodinger equation is:

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right] = E\psi(x,t) \tag{3}$$

$E$ is the energy. It has solutions $\psi_n(x)$ with quantized energies given by:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{4}$$

Where $n = 0, 1, 2, ...$ The analitical solutions of $\psi_n(x)$ are given by the Hermite polinomials. The first ones can be found at [1]. Since the first one, $n = 0$, is gonna be extensively used in this project, here it is:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} exp\left(-\frac{m\omega x^2}{2\hbar}\right) \tag{5}$$

These solutions are, as the name says, solutions for the time independent equation, but it can be added a complex exponential to $\psi$, this adds a momentum and a temporal evolution to it.

$$\psi_n(x,t) = \psi_n(x)e^{ik_0 x} \tag{6}$$

Here $k_0$ are the wave number. The period of oscillation is:

$$T = \frac{2\pi}{\omega} \tag{7}$$

In quantum mechanics we work with operators such as energy, position, momentum, etc... The expected value of an operator is what we measure in quantum systems. The expected value of an operator $O$ is given by:

$$\langle O \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,t)\left[O\psi(x,t)\right]dx}{\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx} \tag{8}$$

Where $[O\psi(x,t)]$ represents the action of O in $\psi$. The operators that had been used in this project are:

Position:

$$\langle X \rangle = x \tag{9}$$

Momentum:

$$\langle P \rangle = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{10}$$

Energy:

$$\langle E \rangle = \hat{H} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right] \tag{11}$$

$H$ is the hamiltonian of the system.

It was also estudied the Ehrenfest theorem. The theorem combines the time derivative of a expected value of an operator and the expected value of his comutative with the hamiltonian of the system [2], that is:

$$\frac{d}{dt}\langle O \rangle = \frac{1}{i\hbar}\langle [O,H] \rangle + \left\langle \frac{\partial O}{\partial t} \right\rangle \tag{12}$$

Having that in mind we can relate the position $x$ and the momentum $p$ by:

$$m\frac{d}{dt}\langle x \rangle = \langle p \rangle \tag{13}$$

And, in the same way, $p$ and the potential $V$:

$$\frac{d}{dt}\langle p \rangle = \left\langle -\frac{\partial}{\partial x}V(x) \right\rangle \tag{14}$$

# 2 Numerical simulation description and results

## 2.1 Runge-Kutta method

To made this simulations it was used the Runge-Kutta of order two method. The $RK2$ is a iterative numerical method to solve diferential equations approximately. It's sort of a upgrade of the Euler method, being that this last one doesn't hold the normalization of the functions, which is a very important condition in many systems. While the Euler method utilizes one step to calculate the next iteration, the RK2 method does the same calculation in two steps, one in mid-term between $n$ and $n+1$.

Given a variable $x(t)$ the method $RK2$ is:

$$k_1^x = \frac{\partial x(t)}{\partial t}\Delta t \tag{15}$$

$$x(t + \Delta t/2) = x_{int} = x(t) + k_1^x/2 \tag{16}$$

$$k_2^x = \frac{\partial x(t + \Delta t/2)}{\partial t}\Delta t \tag{17}$$

$$x(t + \Delta t) = x(t) + k_2^x \tag{18}$$

This can be done for all variables in the system. To do a derivative of a function had been used the diference between the next and the last point of this function. To implement this process and solve the Schrodinger equations it was used the program Octave [3].

## 2.2 Results

The values that were used in this simulation are $m = 1$, $\hbar = 1$ and $\omega = 50$. A parameter defined as $r \equiv dt/(2dx^2)$ which is used to determine the spatial interval $dx$ has the value 0.075, the time interval is $dt = 10^{-4}$. A smaller $r$ implies a shift in the energy (decrease), which we do not want, a bigger $r$ implies that the energy and the normalization both go to infinity, whice we also do not want. These problems aren't totally corrected by a change in $dt$. So these are good values for these kind of simulations.

The normalization must hold for every condition, this is checked by a graphic of nomalization of $\psi$ by time:

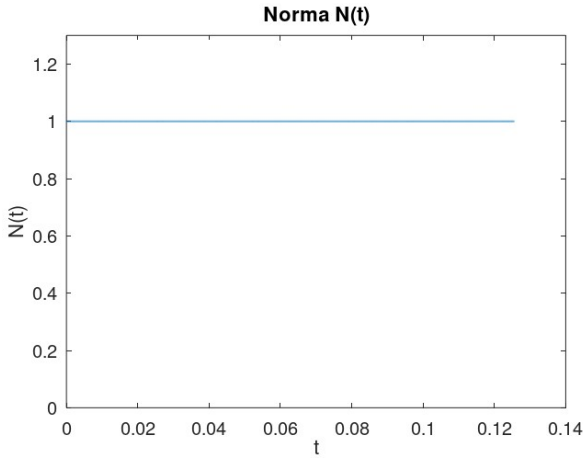


Figure 1: Normalization of $\psi$.

With the normalization in order are obtained the form of $|\psi|^2$ and the potential $V$, in that case $\psi_0$:

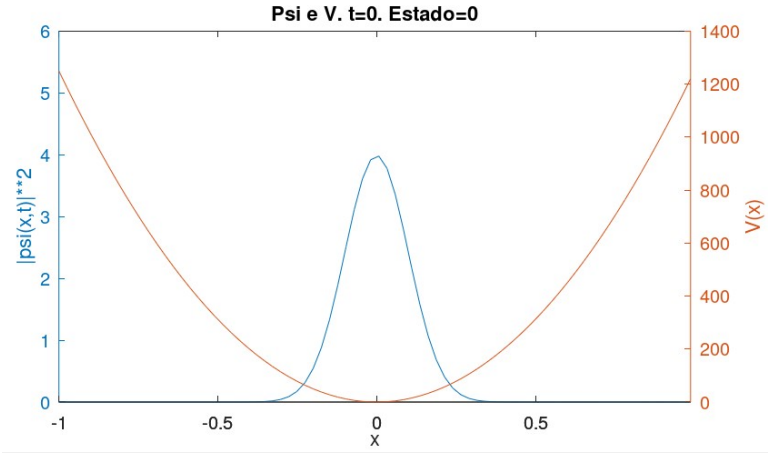


Figure 2: Form of $|\psi_0|^2$ and the potential V.

The expected value of energy (calculated with equation 11) in comparison with the allowed values of energy for the system (equation 4):

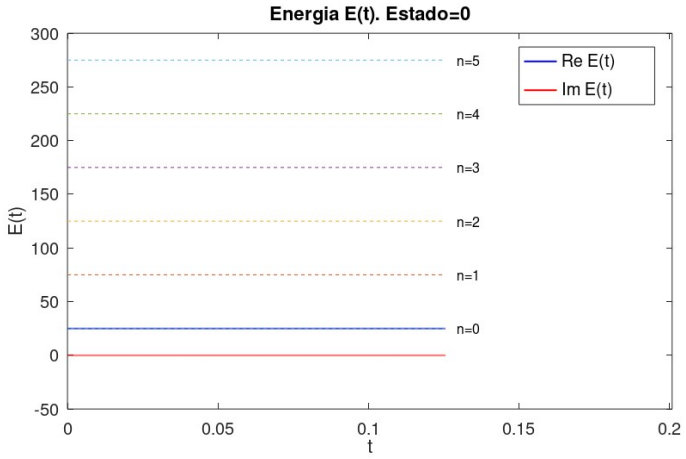


Figure 3: Calculated energies and the expected value of energy for $\psi_0$.

The same comparison with other orders of $\psi$:

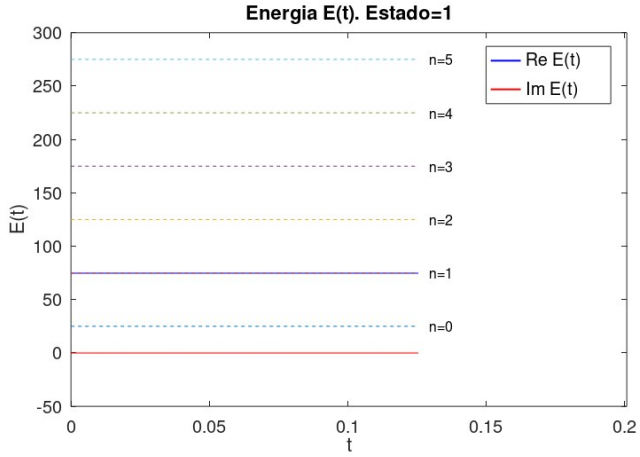


Figure 4: Calculated energies and the expected value of energy for $\psi_1$.

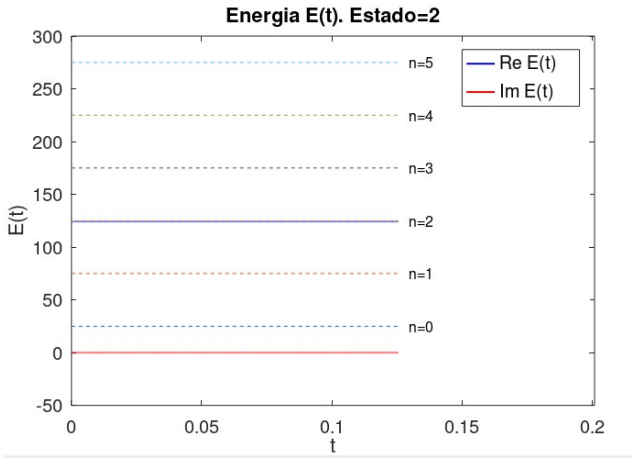


Figure 5: Calculated energies and the expected value of energy for $\psi_2$.

The expected values of energy are exactly the same as the prediction. The normalization holds for all cases. As a complex exponential is added to $\psi$ (equation 6) it's possible to observe the evolution of $\psi_0(x,t)$ in time ($k_0 = 20$).

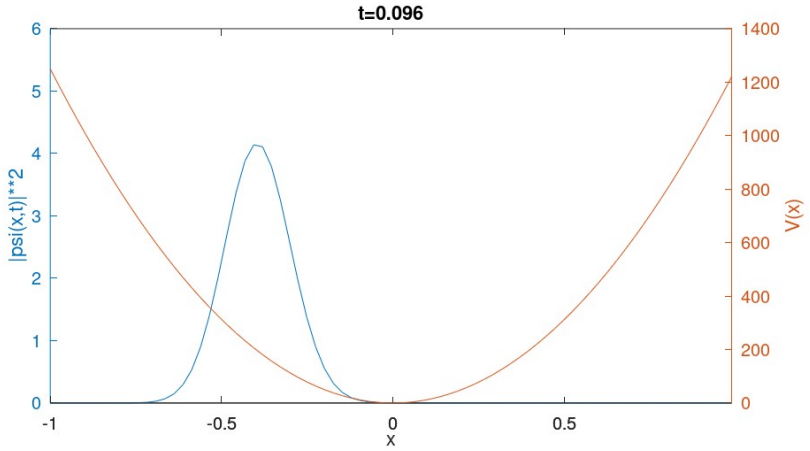


Figure 6: A frame of the animation of $|\psi|^2$ in a given time.

This alterates the values of energy, because, as said, this adds momentum to $\psi$. With this, the value of energy for $\psi_0$ with $k_0 = 20$:

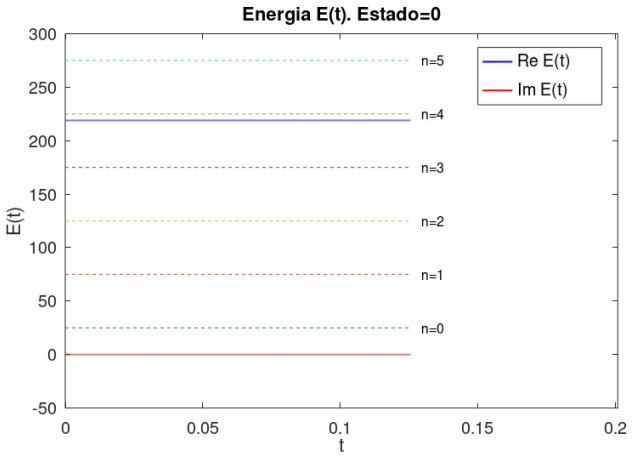


Figure 7: Calculated energies and the expected value of energy for $\psi_0 e^{ik_0 x}$.

We are dealing with the ground state ($n = 0$) but the energy is almost the same as the state of $n = 4$, this difference is caused by the momentum of $\psi$.

To show the oscillation of the system it is presented a graphic of the expected value of $x$ in function of time for one oscillation (equation 7), again with $k_0 = 20$:

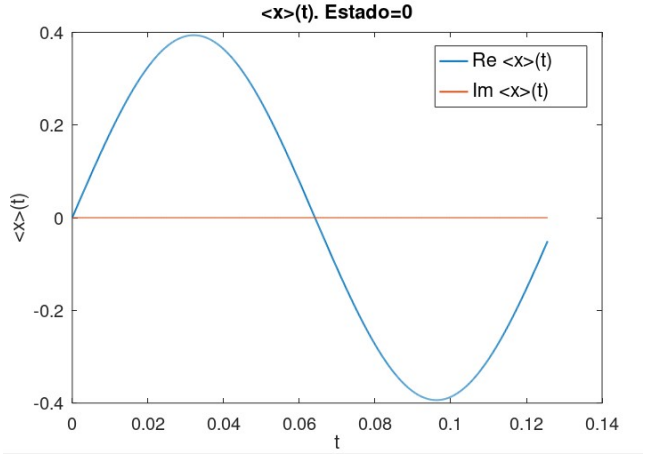


Figure 8: Expected value of $x$ in function of time for $\psi_0 e^{ik_0 x}$.

Now is possible to verificate whether the Ehrenfest theorem (equation 12), in special the equations 13 and 14, are valid.

The equation 13:

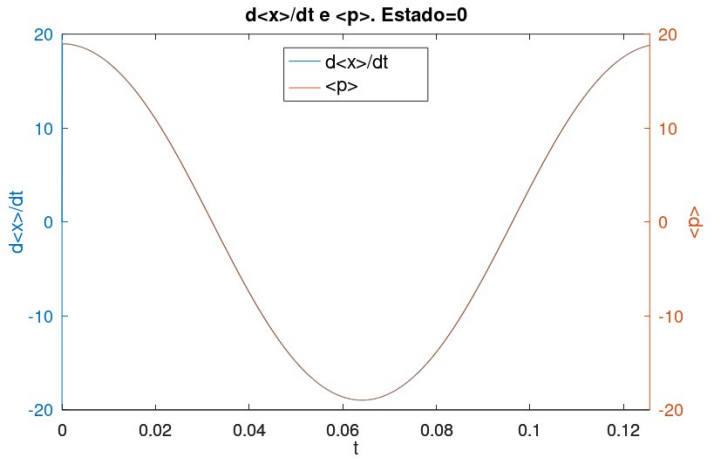


Figure 9: Derivative of the expected value of $x$ times the mass and the expected value of $p$ for $\psi_0 e^{ik_0 x}$.

The two curves are one above another showing that the simulation represents with great form the oscillation of the system.

The equation 14:

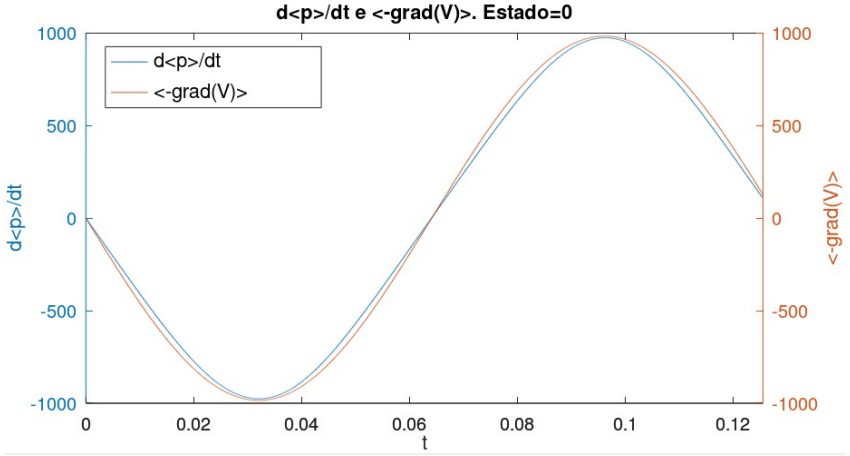


Figure 10: Derivative of the expected value of $p$ and the expected value of the derivative, in relation to the position, of the potential $V(x)$ for $\psi_0 e^{ik_0 x}$.

In this case the two lines have a little divergence that can be adressed as fluctuations by the numerical approach. In general the Ehrenfest theorem is valid with great precision in this simulation.

Another thing that it's interesting it's something called the correspondence principle, as it can be seen in the format of $|\psi|^2$, according you increase $n$ the probability distribuction $|\psi|^2$ increases in the corners and decreases in the center, as it tends to the behavior of a classic oscillator according the raise of $n$. As a classical oscillator spendes more time in the corners than in the center [1].

# 3 User's manual

It's a very easy program to use, in lines 13 to 22 are the parameters that can be modified by the user. "evolu_temp" can be choosen as "Sim" or "Nao", if "Sim" is choosed the temporal evolution of psi (equation 6) is added, otherwise it isn't. $k_0$ is the wave number aready cited, $m$ is the mass, $e$ it's the state wanted, that means $n = 0, 1, ...$ The program allows $n$ from 0 to 3. $w$ is the frequency $\omega$. $r$ is the parametrer cited in the beggining of subsection 2.2 and it determines (along with the time definition $dt$) the spatial definition $dx$. $T$ is the period, equation 7, and it's a suggestion of the final time of the simulation, $t$ is the vector of time, $t = intitial\,time\ : dt :\ final\,time$.

The program then starts some necessary vectors, parameters, and the initial conditions, like $\psi$ and her's temporal evolution. He thens calculate the evolution of $\psi$ in time.

In sequence it calculates and plot graphics for the normalization, energy and form of the probability $|\psi|^2$, in this order. If "evolu_temp" is choosen as "Sim" it then also calculates the expected values of the Ehrenfest theorem, like $< x >$ and $< p >$, and it's derivatives. And then plots the graphics to check the theorem. In the last graphic it shows an animation of $|\psi|^2$ in time.

# 4 Conclusion

The program calculates everything we need to study the properties that we wanted with a very reasonable time, around some minutes for a period of oscillation, which allows us to do multiple simulations for every $n$.

The results are compatible with what we expected, the form of psi, her evolution, the normalization, the energies, the Ehrenfest theorem and the correspondence principle.

# References


[1] Carl R. Nave. Quantum harmonic oscillator: Wavefunctions, 2016. URL `http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hosc5.html#c1`. [Online; accessed 18-June-2020].

[2] Wikipédia. Teorema de ehrenfest — wikipédia, a enciclopédia livre, 2013. URL

https://pt.wikipedia.org/w/index.php?title=Teorema_de_Ehrenfest&oldid=36785830. [Online; accessed 18-Junho-2020].

[3] John W. Eaton, David Bateman, Søren Hauberg, and Rik Wehbr ing. *GNU Octave version 5.2.0 manual: a high-level interactive langua ge for numerical computations*, 2020. URL https://www.gnu.org/software/octave/doc/v5.2.0/.