QCQT-QE5

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1 Preface

This project is done in the context of the course ”QE5 - Applied Quantum Mechanics” of the ”MSC in Quantum Computing and Quantum Technologies - DUTH” with the professor Mr. Emmanuel Paspalakis.
It is based on the paper **W. S. Nascimento, M. M. de Almeida, and F. V. Prudente (2020), Information and quantum theories: an analysis in one-dimensional systems Eur. J. Phys. 41, 025405** [1] and its purpose is to rederive the calculations and results of this paper.
For some integrals that are difficult to calculate with analytical methods, numerical computation with the Python programming language was used. Python was also used for plotting.
You can find all of the code written for this project in the following repository: `https://github.com/topalidisd-qcqt-duth/qy5-final-project`
There is also a shared jupyter notebook, where you can run the code directly: `https://colab.research.google.com/drive/1kDE7-M03_AQoUVLvay95XDmAfzskEnlT?usp=sharing`

2 Introduction

The field of information theory, is concerned about replicating at a destination point, a message transmitted from a point of origin through a channel. The quantity that measures the amount of information generated in a message by a continuous information source is the Shannon entropy:

$$S(p(x)) = -\int_{-\infty}^{+\infty} p(x)\log_2 p(x)\,dx$$
$$\text{with}\, p(x) \,\text{the probability density}$$

Note that the base of the logarithm represents the unit of information. For example, in the expression above we use base 2, so the unit is the bit.

3 Position and momentum representation in quantum mechanics

The wavefunction in position representation is $\psi(x) = \langle x \,|\, \psi\rangle$
In order to move to the momentum representation, we need the transformation function $\langle x \,|\, p\rangle$, such as:

$$\psi(x) = \int \langle x \,|\, p\rangle \psi(p)\,dx$$

with $\psi(p)$ being the wavefunction in the momentum representation.
It is:

$$\langle p \,|\, x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-\dfrac{ipx}{\hbar}}$$

So:

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\dfrac{ipx}{\hbar}} \psi(x)\,dx$$

We can say that $\psi(p)$ is the Fourier transform of $\psi(x)$

Knowing this, we can name $\rho(x) = |\psi(x)|^2$ the probability density in position space and $\gamma(p) = |\tilde{\psi(p)}|^2$ the probability density in momentum space, with $\tilde{\psi(p)}$ being the Fourier transform of $\psi(x)$. Note that both probability densities are normalized, so:

$$\int \rho(x)\, dx = 1$$
$$\int \gamma(p) dp = 1$$

4 Information entropy

Having the representation of the wavefunction in hand, we can define the information entropy as:

$$S_x = -\int \rho(x) \ln(a_0 \rho(x))\, dx\,, \text{ in position space}$$
$$S_y = -\int \gamma(p) \ln(\frac{\hbar}{a_0}\gamma(p)) dp\,, \text{ in momentum space}$$

Then the sum of the two entropies can be defined as:

$$\begin{aligned}
S_t = S_x + S_y &= -\int \rho(x) \ln(a_0 \rho(x))\, dx - \int \gamma(p) \ln(\frac{\hbar}{a_0}\gamma(p)) dp \\
&= -\int \rho(x) \ln(a_0 \rho(x))\, dx - \int \gamma(p) \big[\ln(\frac{\hbar}{a_0}) + \ln(\gamma(p)) \big] dp \;\; \text{Using } \ln(ab) = \ln(a) + \ln(b) \\
&= -\int \rho(x) \ln(a_0 \rho(x))\, dx - \ln(\frac{\hbar}{a_0}) \underbrace{\int \gamma(p)\, dp}_{=1, \text{ since } \gamma(p) \text{ is normalized}} - \int \ln(\gamma(p))\gamma(p) dp \\
&= -\int \rho(x) \ln(a_0 \rho(x))\, dx - \ln(\frac{\hbar}{a_0}) - \int \gamma(p) \ln(\gamma(p)) dp \\
&= -\iint \rho(x)\gamma(p) \big[\ln(a_0 \rho(x)) + \ln(\gamma(p)) + \ln(\frac{\hbar}{a_0}) \big] dx\, dp \\
&= -\iint \rho(x)\gamma(p) \ln(a_0 \frac{\hbar}{a_0} \rho(x)\gamma(p)) dx\, dp \;\; \text{Using } \ln(ab) = \ln(a) + \ln(b) \\
&= -\iint \rho(x)\gamma(p) \ln(\hbar \rho(x)\gamma(p)) dx\, dp
\end{aligned}$$

We can see that each entropy taken separately decreases without bound when the corresponding probability density is becoming more and more concentrated i.e. when the information is increasing.
The total entropy though, has a bound, as shown in [1] and proven in [2]. This bound is:

$$S_t \geq (1 + \ln(\pi))$$

5 Entropy as a measure of uncertainty in quantum mechanics

In quantum mechanics, the expectation values of position and momentum are:

$$\langle x \rangle = \int x \rho(x) dx$$
$$\langle p \rangle = \int p \gamma(p) dp$$

We also know that the respective uncertainties are calculated as:

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$
$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

and that Δx and Δp adhere to the **Heisenberg uncertainty principle**:

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

The entropies S_x and S_y can also be used to measure uncertainty, but with different characteristics from Δx and Δp. The entropic uncertainty relationship $S_t \geq (1 + \ln(\pi))$ is considered a stronger version of the Heisenberg uncertainty principle in the sense that we can derive the later from the former [1].
In the following sections, we will examine how the entropy behaves as a measure of uncertainty in actual quantum mechanical systems. Specifically, we will study the 1-D harmonic oscillator and the infinite potential well.

6 Harmonic oscillator

The harmonic oscillator potential is:

$$V(x) = \frac{1}{2} m\omega^2 x^2 \text{ with } \omega = \sqrt{\frac{\kappa}{m}}$$

The eigenenergies are:

$$E_n = \hbar\omega(n + \frac{1}{2}) \, , n \in \mathbb{Z}$$

The eigenfunctions in the position representation are:

$$\psi_n(x) = \frac{1}{\sqrt{2^n \cdot n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} H_n(\sqrt{\frac{m\omega}{\hbar}} x) e^{-\frac{m\omega x^2}{2\hbar}}$$

$$\text{with } H_n(\sqrt{\frac{m\omega}{\hbar}} x) \text{ the respective Hermite polynomial}$$

The eigenfunctions in the momentum representation are (as seen in [4] Eq. 4.48):

$$\psi_n(p) = \frac{1}{\sqrt{2^n \cdot n!}} \left(\frac{1}{\pi m\omega\hbar}\right)^{\frac{1}{4}} H_n(\frac{1}{\sqrt{m\omega\hbar}} x) e^{-\frac{p^2}{2m\omega\hbar}}$$

Then we have:

$$\begin{aligned}
\rho(x) &= |\psi(x)|^2 \\
&= \left| \frac{1}{\sqrt{2^n \cdot n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} H_n(\sqrt{\frac{m\omega}{\hbar}} x) e^{-\frac{m\omega x^2}{2\hbar}} \right|^2 \\
&= \frac{1}{2^n \cdot n!} \sqrt{\frac{m\omega}{\pi\hbar}} H_n^2(\sqrt{\frac{m\omega}{\hbar}} x) e^{-\frac{m\omega x^2}{\hbar}} \\
&= \frac{a}{2^n \cdot n!} \frac{1}{\sqrt{\pi}} H_n^2(ax) e^{-a^2 x^2} \quad \text{, with } a = \sqrt{\frac{m\omega}{\hbar}}
\end{aligned}$$

and

$$\begin{aligned}
\gamma(p) &= |\psi(p)|^2 \\
&= \Big| \frac{1}{\sqrt{2^n \cdot n!}} \Big(\frac{1}{\pi m \omega \hbar}\Big)^{\frac{1}{4}} H_n\big(\frac{1}{\sqrt{m\omega\hbar}} p\big) e^{-\frac{p^2}{2m\omega\hbar}} \Big|^2 \\
&= \frac{1}{2^n \cdot n!} \frac{1}{\sqrt{\pi m \omega \hbar}} H_n^2\big(\frac{1}{\sqrt{m\omega\hbar}} p\big) e^{-\frac{p^2}{m\omega\hbar}} \\
&= \frac{b}{2^n \cdot n!} \frac{1}{\sqrt{\pi}} H_n^2(bp) e^{-b^2p^2} \quad \text{, with } b = \frac{1}{\sqrt{m\omega\hbar}}
\end{aligned}$$

Knowing $\rho(x)$ and $\gamma(p)$, we can obtain general expressions for S_x and S_y:

$$\begin{aligned}
S_x &= -\int_{-\infty}^{+\infty} \rho(x) \ln\Big(a_0 \frac{a}{2^n \cdot n!} \frac{1}{\sqrt{\pi}} H_n^2(ax) e^{-a^2x^2}\Big)\, dx \\
&= -\int_{-\infty}^{+\infty} \rho(x) \Big[\ln\Big(a_0 \frac{a}{2^n \cdot n!} \frac{1}{\sqrt{\pi}}\Big) + \ln\Big(H_n^2(ax) e^{-a^2x^2}\Big)\Big]\, dx \\
&= -\int_{-\infty}^{+\infty} \ln\Big(a_0 \frac{a}{2^n \cdot n!} \frac{1}{\sqrt{\pi}}\Big) \rho(x)\, dx - \int_{-\infty}^{+\infty} \ln\Big(H_n^2(ax) e^{-a^2x^2}\Big) \frac{a}{2^n \cdot n!} \frac{1}{\sqrt{\pi}} H_n^2(ax) e^{-a^2x^2}\, dx \\
&= -\ln\Big(a_0 \frac{a}{2^n \cdot n!} \frac{1}{\sqrt{\pi}}\Big) \underbrace{\int_{-\infty}^{+\infty} \rho(x)\, dx}_{= 1, \text{ since } \rho(x) \text{ is normalized}} - \frac{a}{2^n \cdot n!} \frac{1}{\sqrt{\pi}} \Big[2 \int_0^{\infty} \ln\Big(H_n^2(ax)\Big) H_n^2(ax) e^{-a^2x^2} dx - \int_{-\infty}^{+\infty} a^2x^2 H_n^2(ax) e^{-a^2x^2}\, dx \Big] \\
&= -\ln\Big(a_0 \frac{a}{2^n \cdot n!} \frac{1}{\sqrt{\pi}}\Big) - \frac{a}{2^n \cdot n!} \frac{1}{\sqrt{\pi}} \Big[2 \int_0^{\infty} \ln\Big(H_n^2(ax)\Big) H_n^2(ax) e^{-a^2x^2} dx - a^2 \int_{-\infty}^{+\infty} x^2 H_n^2(ax) e^{-a^2x^2}\, dx \Big]
\end{aligned}$$

$$\begin{aligned}
S_p &= -\int_{-\infty}^{\infty} \gamma(p) \ln\Big(\frac{\hbar}{a_0} \frac{b}{2^n \cdot n!} \frac{1}{\sqrt{\pi}} H_n^2(bp) e^{-b^2p^2}\Big) dp \\
&= -\int_{-\infty}^{\infty} \gamma(p) \Big[\ln\Big(\frac{\hbar b}{a_0 \cdot 2^n \cdot n!} \frac{1}{\sqrt{\pi}}\Big) + \ln\Big(H_n^2(bp) e^{-b^2p^2}\Big)\Big] dp \\
&= -\int_{-\infty}^{\infty} \ln\Big(\frac{\hbar b}{a_0 \cdot 2^n \cdot n!} \frac{1}{\sqrt{\pi}}\Big) \gamma(p) dp - \int_{-\infty}^{\infty} \ln\Big(H_n^2(bp) e^{-b^2p^2}\Big) \frac{b}{2^n \cdot n!} \frac{1}{\sqrt{\pi}} H_n^2(bp) e^{-b^2p^2} dp \\
&= -\ln\Big(\frac{\hbar b}{a_0 \cdot 2^n \cdot n!} \frac{1}{\sqrt{\pi}}\Big) \underbrace{\int_{-\infty}^{\infty} \gamma(p) dp}_{= 1, \text{ since } \gamma(p) \text{ is normalized}} - \frac{b}{2^n \cdot n!} \frac{1}{\sqrt{\pi}} \Big[2 \int_0^{\infty} \ln\Big(H_n^2(bp)\Big) H_n^2(bp) e^{-b^2p^2} dp - \int_{-\infty}^{\infty} b^2p^2 H_n^2(bp) e^{-b^2p^2} dp \Big] \\
&= -\ln\Big(\frac{\hbar b}{a_0 \cdot 2^n \cdot n!} \frac{1}{\sqrt{\pi}}\Big) - \frac{b}{2^n \cdot n!} \frac{1}{\sqrt{\pi}} \Big[2 \int_0^{\infty} \ln\Big(H_n^2(bp)\Big) H_n^2(bp) e^{-b^2p^2} dp - b^2 \int_{-\infty}^{\infty} p^2 H_n^2(bp) e^{-b^2p^2} dp \Big]
\end{aligned}$$

In order to calculate the entropies for different values of ω and in different states, we will use the **Python** programming language, along with the libraries **numpy** and **sympy**.
You can find all the necessary code for the calculations here: `https://github.com/topalidisd-qcqt-duth/qy5-final-project/tree/main/harmonic-oscillator`
Specifically you will find:

- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/harmonic-oscillator/harmonic_oscillator.py`, which has the general framework for working with the harmonic oscillator.
- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/harmonic-oscillator/ho_ground_state.py`, which can be used to calculate the value of S_x, S_p and S_t for different ω values in the ground state.
- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/harmonic-oscillator/ho_first_excited_state.py`, which can be used to calculate the value of S_x, S_p and S_t for different ω values in the first excited state.

- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/harmonic-oscillator/ho_second_excited_state.py`, which can be used to calculate the value of S_x, S_p and S_t for different ω values in the second excited state.
- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/harmonic-oscillator/ho_probability_density_plot.py`, which can be used to plot the probability densities of $\psi(x)$ and $\psi(p)$ for the ground state, first excited state and second excited state.
- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/harmonic-oscillator/ho_entropies_plot.py`, which can be used to plot the entropies S_x, S_p and the total entropy S_t.

We can use this code to calculate the entropies and uncertainties in specific states.
Note that we use **atomic units** for all of our calculations.
In the table below, we can see the results we obtain for $\omega = 0.06$, $\omega = 0.5$ and $\omega = 1$, in the ground state, first excited state and second excited state.
Those results are the same as in [1].

$\omega = \mathbf{0.06}$

n	$\mathbf{S_x}$	$\mathbf{S_p}$	$\mathbf{S_t}$
1	**2.4791**	**-0.3343**	**2.1447**
2	**2.7494**	**-0.064**	**2.6855**
3	**2.9053**	**0.0919**	**2.9972**

Table 1: Results obtained for the entropies in the case of the harmonic oscillator with $\omega = 0.06$, in the ground state, first and second excited states.

$\omega = \mathbf{0.5}$

n	$\mathbf{S_x}$	$\mathbf{S_p}$	$\mathbf{S_t}$
1	**1.4189**	**0.7258**	**2.1447**
2	**1.6893**	**0.9962**	**2.6855**
3	**1.8452**	**1.1520**	**2.9972**

Table 2: Results obtained for the entropies in the case of the harmonic oscillator with $\omega = 0.5$, in the ground state, first and second excited states.

$\omega = \mathbf{1}$

n	$\mathbf{S_x}$	$\mathbf{S_p}$	$\mathbf{S_t}$
1	**1.0724**	**1.0724**	**2.1447**
2	**1.3427**	**1.3427**	**2.6855**
3	**1.4986**	**1.4986**	**2.9972**

Table 3: Results obtained for the entropies in the case of the harmonic oscillator with $\omega = 1$, in the ground state, first and second excited states.

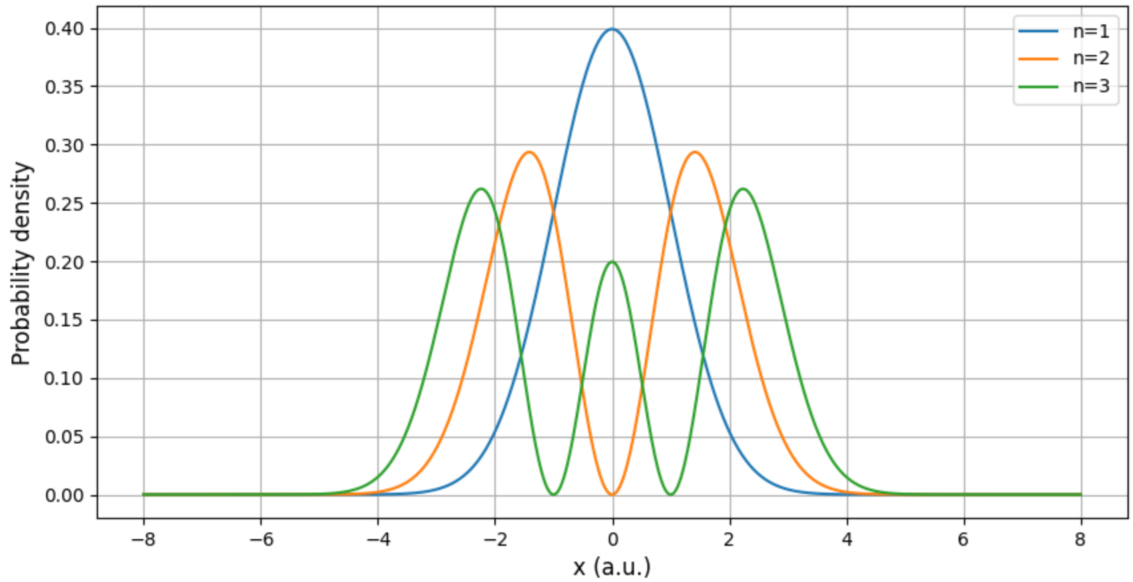

Figure 1: Probability density in position space

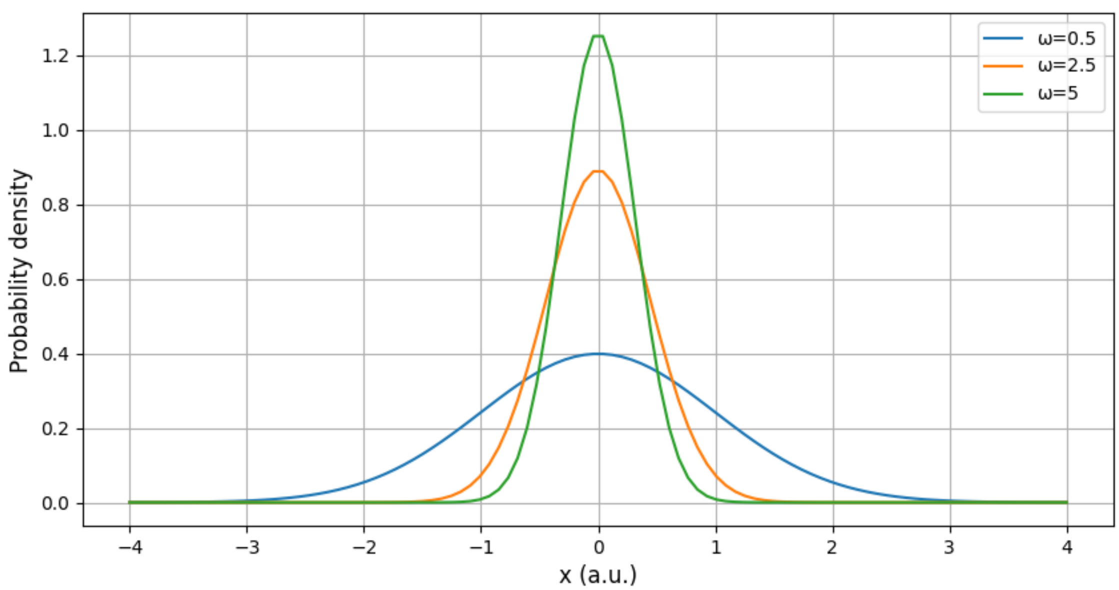

Figure 2: Probability density in position space as a function of ω

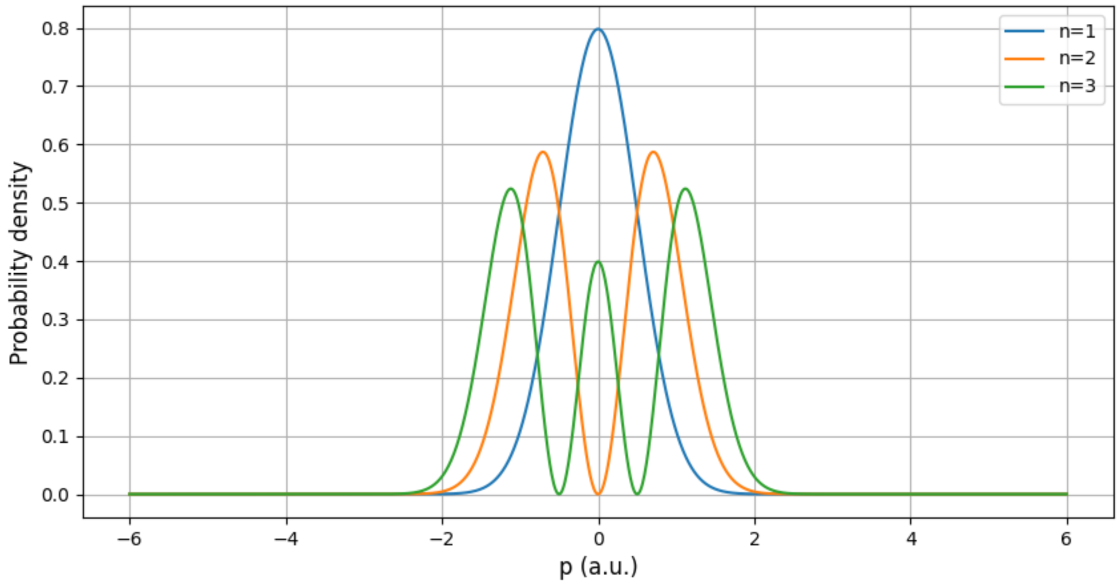

Figure 3: Probability density in momentum space

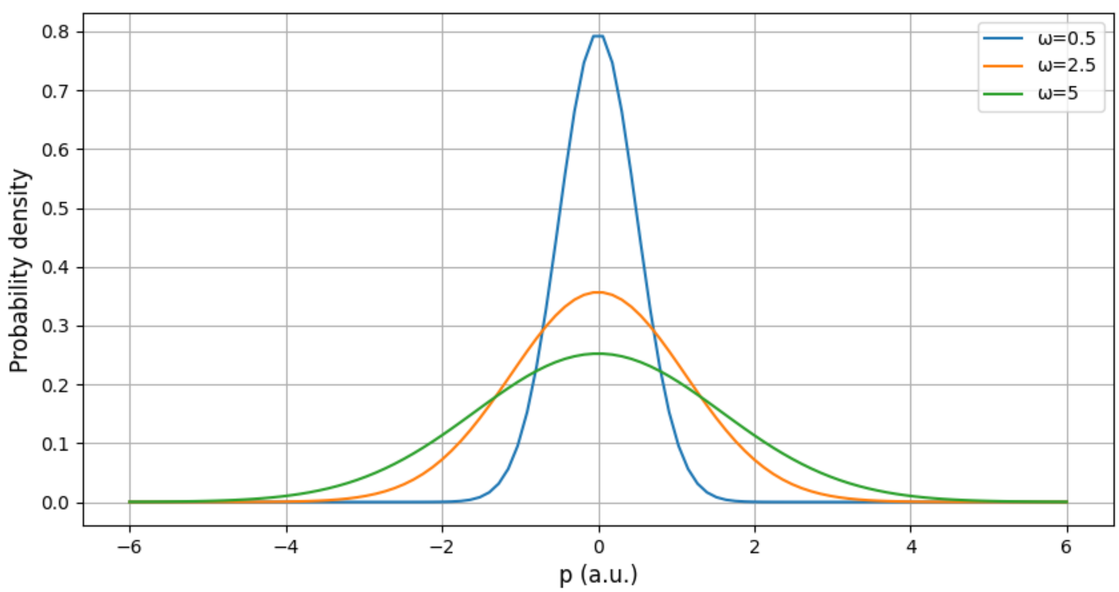

Figure 4: Probability density in momentum space as a function of ω

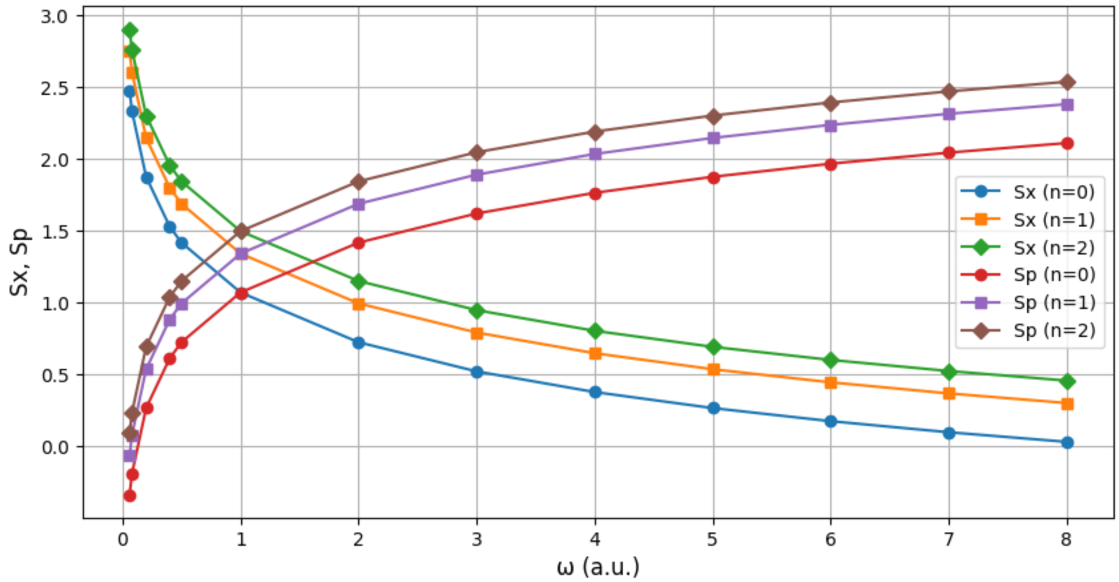

Figure 5: Entropies S_x and S_p as functions of ω

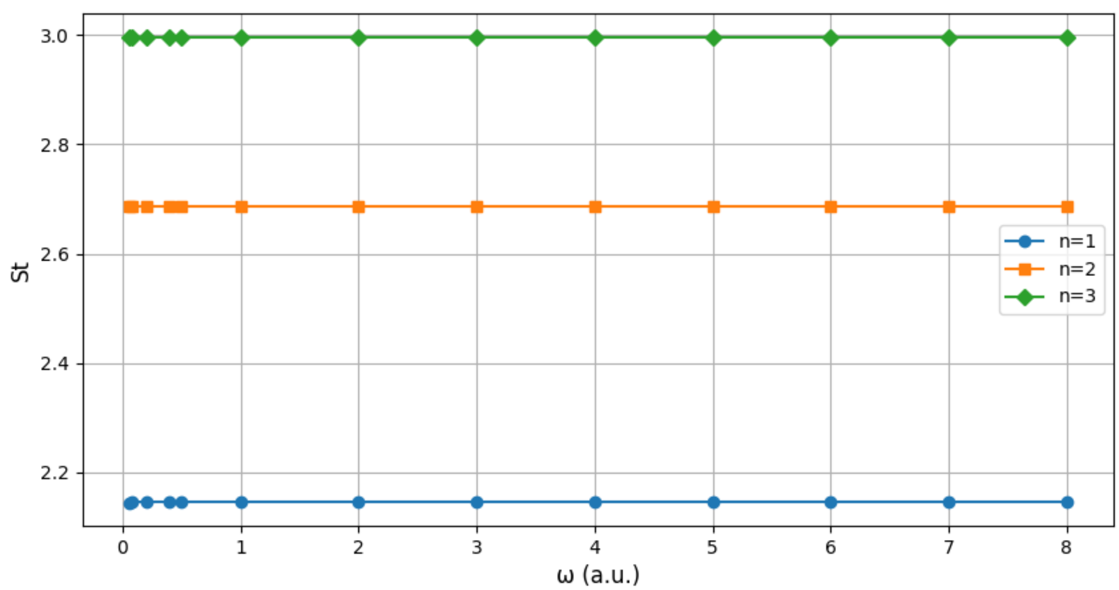

Figure 6: Total entropy S_t as a function of ω

6.1 Observations

Based on the results we obtained for the entropies' values, we can see that S_x and S_p increase, when n increases. This is in accordance with what we see in 1 and 3. The spread of the probability densities also increases when n increases.

The total entropy S_t also exhibits the same behavior, but is independent of ω, so it remains constant in each state of the system.
If we look into the probability densities and the values of the entropies S_x and S_p with respect to ω, we see that increasing values of ω result in increasing probability density spread and entropy for position and decreasing for momentum. This is interpreted as the uncertainty relationship between the two observables. [1]

7 Infinite potential well

The infinite well potential is:

$$V(x) = \begin{cases} 0\,, -L \leq x \leq L \\ \infty\,, x < -L \text{ or } x > L \end{cases}$$

The eigenenergies are:

$$E_n = \frac{\pi^2 \hbar^2}{2mL^2} n^2$$

The eigenfunctions in the position representation are:

$$\psi_n(x) = \frac{1}{\sqrt{L}} \cos(\frac{n\pi x}{2L}) \text{ , for } n \text{ odd}$$
$$\psi_n(x) = \frac{1}{\sqrt{L}} \sin(\frac{n\pi x}{2L}) \text{ , for } n \text{ even}$$

We can find the momentum representation using the Fourier transform relation.

For odd n:

$$\begin{aligned}
\psi_n(p) &= -\frac{1}{\sqrt{2\pi\hbar}}\int_{-L}^{L}\psi_n(x)e^{-ipx/\hbar}dx \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int_{-L}^{L}e^{-ipx/\hbar}\frac{1}{\sqrt{L}}\cos(\frac{n\pi x}{2L})dx \\
&= \frac{1}{\sqrt{2\pi\hbar L}}\int_{-L}^{L}e^{-icx}\cos(bx)dx \text{ We set } c=\frac{p}{\hbar} \text{ and } b=\frac{n\pi}{2L} \\
&= \frac{1}{\sqrt{2\pi\hbar L}}\int_{-L}^{L}e^{-icx}(\frac{e^{ibx}+e^{-ibx}}{2})dx \\
&= \frac{1}{2\sqrt{2\pi\hbar L}}\int_{-L}^{L}e^{-i(c-b)x}+e^{-i(c+b)x}dx \\
&= \frac{1}{2\sqrt{2\pi\hbar L}}\left[\frac{1}{-i(c-b)}e^{-i(c-b)x}\Big|_{-L}^{L}+\frac{1}{-i(c+b)}e^{-i(c+b)x}\Big|_{-L}^{L}\right] \\
&= \frac{1}{2\sqrt{2\pi\hbar L}}\cdot\frac{i}{c^2-b^2}\left[(c+b)e^{-i(c-b)x}\Big|_{-L}^{L}+(c-b)e^{-i(c+b)x}\Big|_{-L}^{L}\right] \\
&= \frac{1}{2\sqrt{2\pi\hbar L}}\cdot\frac{i}{c^2-b^2}\Big[(c+b)(e^{-i(c-b)L}-e^{i(c-b)L})+(c-b)(e^{-i(c+b)L}-e^{i(c+b)L})\Big] \\
&= \frac{1}{2\sqrt{2\pi\hbar L}}\cdot\frac{i}{c^2-b^2}\Big[(c+b)(-2i)\sin((c-b)L)+(c-b)(-2i)\sin((c+b)L)\Big] \\
&= \frac{1}{2\sqrt{2\pi\hbar L}}\cdot\frac{2}{c^2-b^2}\Big[(c+b)\Big(\sin(cL)\cos(bL)-\cos(cL)\sin(bL)\Big)+(c-b)\Big(\sin(cL)\cos(bL)+\cos(cL)\sin(bL)\Big)\Big] \\
&\text{We used } \sin((c+b)a)=\sin(ca+ba)=\sin(ca)\cos(ba)+\cos(ca)\sin(ba) \\
&= \frac{1}{\sqrt{2\pi\hbar L}}\cdot\frac{1}{c^2-b^2}\Big[2c\sin(cL)\cos(bL)-2b\cos(cL)\sin(bL)\Big] \\
&= \frac{1}{\sqrt{2\pi\hbar L}}\cdot\frac{2}{c^2-b^2}\Big[c\sin(cL)\cos(bL)-b\cos(cL)\sin(bL)\Big] \\
&\qquad\qquad\qquad\qquad \text{It is } \sin(\frac{n\pi}{2})=(-1)^{\frac{n-1}{2}} \text{ for odd n, so } -\sin(\frac{n\pi}{2})=(-1)^{\frac{n+1}{2}} \\
&= \frac{1}{\sqrt{2\pi\hbar L}}\cdot\frac{2}{c^2-b^2}\Big[c\sin(cL)\underbrace{\cos(\frac{n\pi}{2})}_{=0\text{ for odd } n}-b\cos(cL)\overbrace{\sin(\frac{n\pi}{2})}\Big] \\
&= \frac{2b(-1)^{\frac{n+1}{2}}}{\sqrt{2\pi\hbar L}(c^2-b^2)}\cos(cL)
\end{aligned}$$

For even n:

$$
\begin{aligned}
\psi_n(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-L}^{L}\psi_n(x)e^{-ipx/\hbar}dx \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int_{-L}^{L}e^{-ipx/\hbar}\frac{1}{\sqrt{L}}\sin(\frac{n\pi x}{2L})dx \\
&= \frac{1}{\sqrt{2\pi\hbar L}}\int_{-L}^{L}e^{-icx}\sin(bx)dx \text{ We set } c=\frac{p}{\hbar} \text{ and } b=\frac{n\pi}{2L} \\
&= \frac{1}{\sqrt{2\pi\hbar L}}\int_{-L}^{L}e^{-icx}(\frac{e^{ibx}-e^{-ibx}}{2i})dx \\
&= \frac{1}{2i\sqrt{2\pi\hbar L}}\int_{-L}^{L}e^{-i(c-b)x}-e^{-i(c+b)x}dx \\
&= \frac{1}{2i\sqrt{2\pi\hbar L}}\Big[\frac{1}{-i(c-b)}e^{-i(c-b)x}\Big|_{-L}^{L}-\frac{1}{-i(c+b)}e^{-i(c+b)x}\Big|_{-L}^{L}\Big] \\
&= \frac{1}{2\sqrt{2\pi\hbar L}}\cdot\frac{1}{c^2-b^2}\Big[(c+b)e^{-i(c-b)x}\Big|_{-L}^{L}-(c-b)e^{-i(c+b)x}\Big|_{-L}^{L}\Big] \\
&= \frac{1}{2\sqrt{2\pi\hbar L}}\cdot\frac{1}{c^2-b^2}\Big[(c+b)(e^{-i(c-b)L}-e^{i(c-b)L})-(c-b)(e^{-i(c+b)L}-e^{i(c+b)L})\Big] \\
&= \frac{1}{2\sqrt{2\pi\hbar L}}\cdot\frac{1}{c^2-b^2}\Big[(c+b)(-2i)\sin((c-b)L)-(c-b)(-2i)\sin((c+b)L)\Big] \\
&= -\frac{1}{2\sqrt{2\pi\hbar L}}\cdot\frac{2i}{c^2-b^2}\Big[(c+b)\Big(\sin(cL)\cos(bL)-\cos(cL)\sin(bL)\Big)-(c-b)\Big(\sin(cL)\cos(bL)+\cos(cL)\sin(bL)\Big)\Big] \\
&\text{We used } \sin((c+b)a)=\sin(ca+ba)=\sin(ca)\cos(ba)+\cos(ca)\sin(ba) \\
&= -\frac{1}{2\sqrt{2\pi\hbar L}}\cdot\frac{2i}{c^2-b^2}\Big[2b\sin(cL)\cos(bL)-2c\cos(cL)\sin(bL)\Big] \\
&= -\frac{1}{\sqrt{2\pi\hbar L}}\cdot\frac{2i}{c^2-b^2}\Big[b\sin(cL)\cos(bL)-c\cos(cL)\sin(bL)\Big] \\
&= -\frac{1}{\sqrt{2\pi\hbar L}}\cdot\frac{2i}{c^2-b^2}\Big[b\sin(cL)\underbrace{\cos(\frac{n\pi}{2})}_{\text{It is }\cos(\frac{n\pi}{2})=(-1)^{\frac{n}{2}}\text{ for even n}}-c\cos(cL)\overbrace{\sin(\frac{n\pi}{2})}^{=0\text{ for even }n}\Big] \\
&= -\frac{2ib(-1)^{\frac{n}{2}}}{\sqrt{2\pi\hbar L}(c^2-b^2)}\sin(cL) \\
&= \frac{2ib(-1)^{\frac{n+2}{2}}}{\sqrt{2\pi\hbar L}(c^2-b^2)}\sin(cL)
\end{aligned}
$$

In order to calculate the entropies for different widths of the infinite potential well and in different states, we will use the **Python** programming language, along with the libraries **numpy** and **sympy**.
You can find all the necessary code for the calculations here: `https://github.com/topalidisd-qcqt-duth/qy5-final-project/tree/main/infinite-square-well`
Specifically you will find:

- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/infinite-square-well/infinite_square_well.py`, which has the general framework for working with the infinite square well.
- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/infinite-square-well/isw_ground_state.py`, which can be used to calculate the value of S_x, S_p and S_t for different L values in the ground state.
- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/infinite-square-well/isw_

`first_excited_state.py`, which can be used to calculate the value of S_x, S_p and S_t for different L values in the first excited state.

- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/infinite-square-well/isw_second_excited_state.py`, which can be used to calculate the value of S_x, S_p and S_t for different L values in the second excited state.
- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/infinite-square-well/isw_probability_density_plot.py`, which can be used to plot the probability densities of $\psi(x)$ and $\psi(p)$ for the ground state, first excited state and second excited state.
- `https://github.com/topalidisd-qcqt-duth/qy5-final-project/blob/main/infinite-square-well/isw_entropies_plot.py`, which can be used to plot the entropies S_x, S_p and the total entropy S_t.

We can use this code to calculate the entropies and uncertainties in specific states.
Note that we use **atomic units** for all of our calculations.
In the table below, we can see the results we obtain for $L = 0.05$, $L = 0.25$ and $L = 1$, in the ground state, first excited state and second excited state.
Those results are the same as in [1]. The only difference is that, they calculate the entropies as functions of the whole width of the potential well, while we use half of the width (the parameter L). So a width $r_c = 0.1000$ in [1] corresponds to $L = 0.05$ in our case.

L = 0.05

n	$\mathbf{S_x}$	$\mathbf{S_p}$	$\mathbf{S_t}$
1	**-2.6094**	**4.8215**	**2.2120**
2	**-2.6094**	**5.2164**	**2.6070**
3	**-2.6094**	**5.3625**	**2.7531**

Table 4: Results obtained for the entropies in the case of the infinite potential well with $L = 0.05$, in the ground state, first and second excited states.

L = 0.25

n	$\mathbf{S_x}$	$\mathbf{S_p}$	$\mathbf{S_t}$
1	**-1.000**	**3.2120**	**2.2120**
2	**-1.000**	**3.6070**	**2.6070**
3	**-1.000**	**3.7531**	**2.7531**

Table 5: Results obtained for the entropies in the case of the infinite potential well with $L = 0.25$, in the ground state, first and second excited states.

L = 1

n	$\mathbf{S_x}$	$\mathbf{S_p}$	$\mathbf{S_t}$
1	**0.3863**	**1.8257**	**2.2120**
2	**0.3863**	**2.2207**	**2.6070**
3	**0.3863**	**2.3668**	**2.7531**

Table 6: Results obtained for the entropies in the case of the infinite potential well with $L = 1$, in the ground state, first and second excited states.

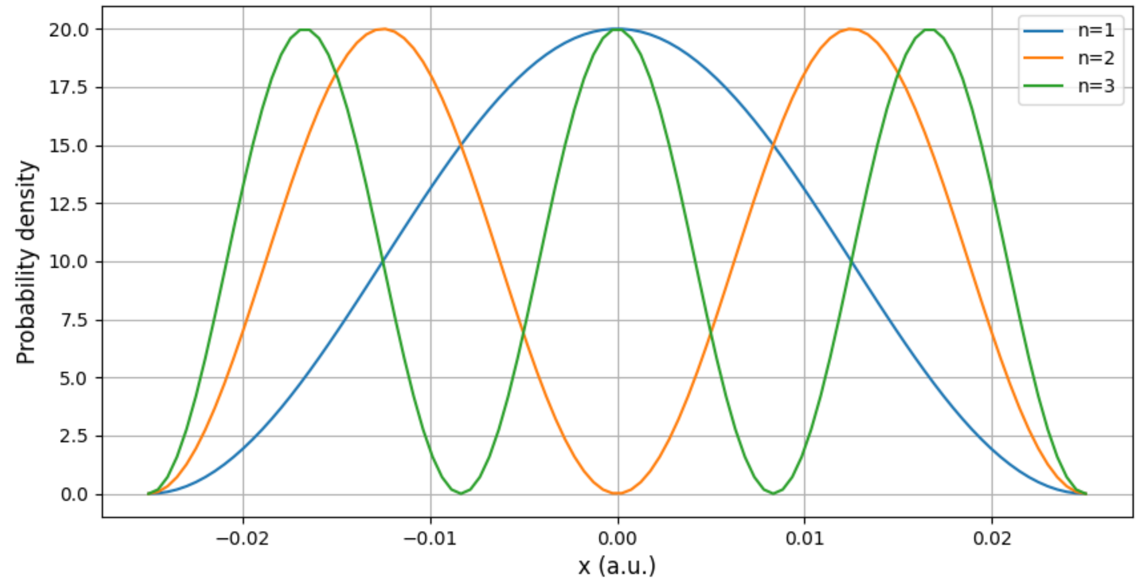

Figure 7: Probability density in position space

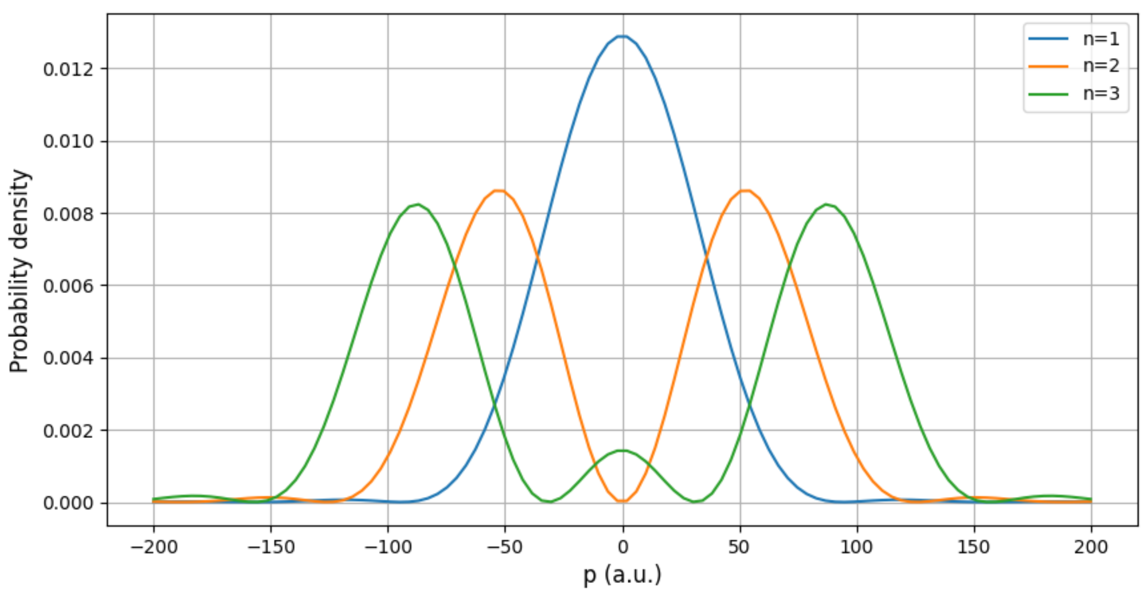

Figure 8: Probability density in momentum space

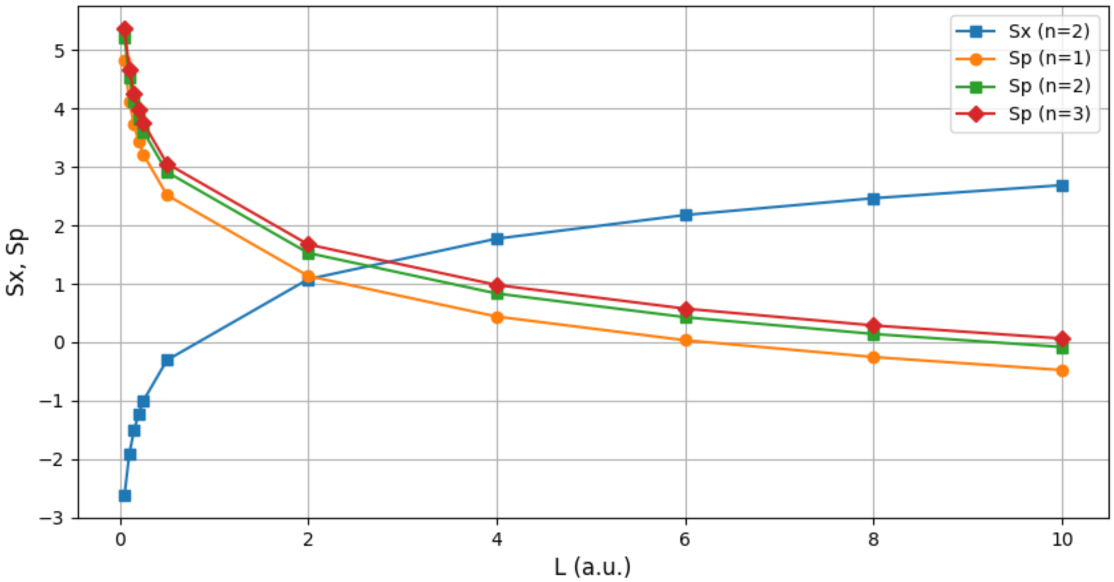

Figure 9: Entropies S_x and S_p as functions of L

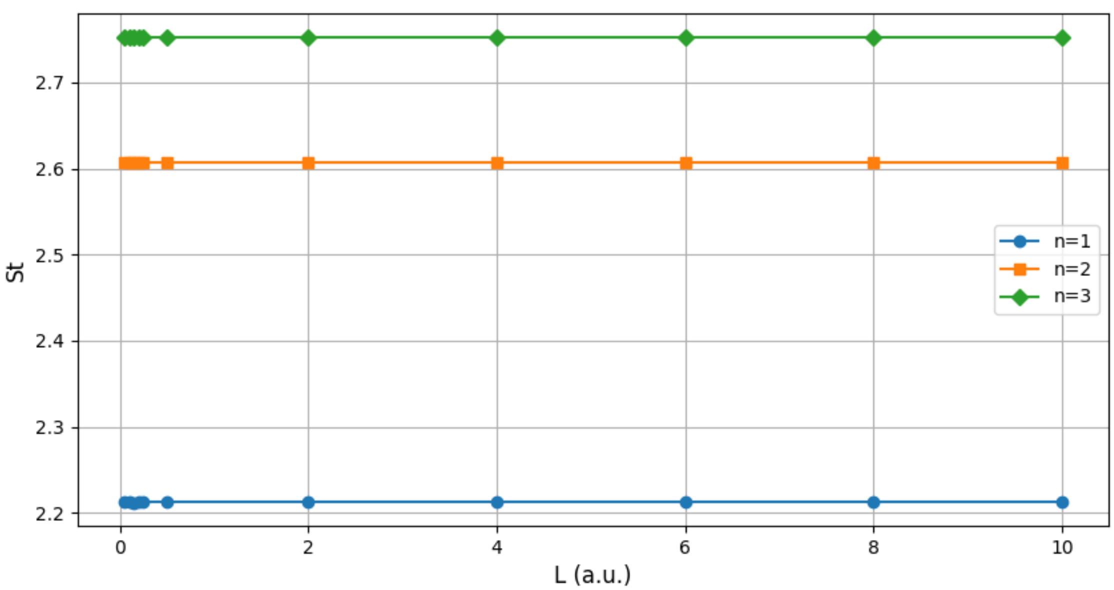

Figure 10: Total entropy S_t as a function pf L

7.1 Observations

Based on the results we obtained for the entropies' values, we can see that we have equal values of S_x for all states, for a given L. On the other hand the value of S_p increases in higher energy states (higher n).
We can also observe that the value of S_x decreases when confinement becomes stronger (lower L), along with the uncertainty in the particle's location. In contrast, the value of S_p increases when confinement becomes stronger.

These results indicate once again that the entropies S_x and S_p represent an measure of position and momentum uncertainty respectively. [1]
Regarding the value of the total entropy S_t, it is independent of L and remains constant in each energy state, but increases between them, as the energy increases itself.

8 Conclusions

In this project we rederived the calculations and results presented in **W. S. Nascimento, M. M. de Almeida, and F. V. Prudente (2020), Information and quantum theories: an analysis in one-dimensional systems Eur. J. Phys. 41, 025405** [1].
The results indicate that information entropies cam be used as an alternative measure of uncertainty for position and momentum in quantum mechanical systems, instead of the classical standard deviations. They also impose an new total uncertainty limit that is stronger that the Heisenberg uncertainty principle.
Specifically, we verifier the above by examining the one dimensional harmonic oscillator and the infinite square well, by calculating the entropies for the ground state, first excited state and second excited state in each system separately.
In the harmonic oscillator case, we observer that the value of S_x increases and the value of S_p decreases when ω reduces.
For the infinite square well, we observed values of S_x that are equal for all three quantum states and that decrease when the confinement becomes stronger (smaller L). The values of S_p on the other hand increase with higher n and stronger confinement.
For both systems, the total entropy S_t remained the same for each state and took its smallest value in the ground state.

References

[1] W. S. Nascimento, M. M. de Almeida, and F. V. Prudente (2020), Information and quantum theories: an analysis in one-dimensional systems Eur. J. Phys. 41, 025405

[2] Bialynicki-Birula I and Mycielski J (1975), Uncertainty relations for information entropy in wave mechanics Commun. Math. Phys

[3] Nouredine Zettili, Quantum Mechanics Concepts and Applications Second Edition

[4] Charles E. Burkhardt · Jacob J. Leventhal, Foundations of Quantum Physics