Computational Physics - Exam Exercise

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Quantum harmonic oscillator

Introduction

Analogous to the classical harmonic oscillator the quantum harmonic oscillator describes a system consisting of a particle in a potential of the form:

$$V(x) = \frac{1}{2} m\omega^2 x^2$$

It gains it's relevance as the first approximation of any potential close to a stable equilibrium point.
The Hamiltonian in full reads:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2}$$

And the Schrödinger equation then follows:

$$i\hbar \frac{\partial}{\partial t}\Phi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}x^2\right)\Phi(x,t)$$

Throughout the rest of this report, is is assumed that: $m = \hbar = 1$:

$$i \frac{\partial}{\partial t}\Phi(x,t) = \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{\omega^2}{2}x^2\right)\Phi(x,t)$$

The initial conditions will be an arbitrary guassian wave packet:

$$\Phi(x, t=0) = \left(\pi\sigma^2\right)^{-1/4} \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right)$$

The goal of the simulation is to observe the time evolution of these gaussian wave packets with different parameter sets ω, σ, x_0 by using the product formula approach to solve the time-dependent Schrödinger equation numerically. Specifically the time evolution of the expectation value of the position operator $\langle \hat{x} \rangle = \langle \Phi | \hat{x} | \Phi \rangle$ and it's variance $(\Delta x)^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$ are of interest.

Analytical considerations

First a special set of states, the coherent states of the quantum harmonic oscillator, is considered:

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

These states, as will be obvious later, correspond to $\sigma = 1$, $x_0 \neq 0$, ergo represent displaced gaussians with a width equal to the width of the ground state.

Among other ways the coherent states can be defined as the eigenstates of the annihilation operator (the “down” ladder operator):

$$
\begin{aligned}
a\left\langle \alpha \right\rangle =& \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} a \left| n \right\rangle \\
=& \sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \sqrt{n} \left| n-1 \right\rangle \\
=& \sum_{n=1}^{\infty} \frac{\alpha \sqrt{n}}{\sqrt{n}} \frac{\alpha^{n-1}}{\sqrt{(n-1)!}} \left| n-1 \right\rangle \\
=& \alpha \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \left| n \right\rangle = \alpha \left| \alpha \right\rangle
\end{aligned}
$$

using the properties of the ladder operators of the harmonic oscillator:

$$
\begin{aligned}
a \left| n \right\rangle &= \sqrt{n} \left| n-1 \right\rangle \\
a \left| 0 \right\rangle &= 0 \\
a^\dagger \left| n \right\rangle &= \sqrt{n+1} \left| n+1 \right\rangle
\end{aligned}
$$

The position operators can be written using the ladder operators:

$$
\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \left(a + a^\dagger\right) = \sqrt{\frac{1}{2\omega}} \left(a + a^\dagger\right)
$$

The mean of the position operator can then be easily calculated:

$$
\begin{aligned}
\langle \alpha | \hat{x} | \alpha \rangle &= \frac{1}{\sqrt{2\omega}} \langle \alpha | a + a^\dagger | \alpha \rangle \\
&= \frac{1}{\sqrt{2\omega}} \left(\langle \alpha | a | \alpha \rangle + \langle \alpha | a^\dagger | \alpha \rangle \right) \\
&= \frac{1}{\sqrt{2\omega}} \left(\langle \alpha | a | \alpha \rangle + \langle \alpha | a | \alpha \rangle^* \right) \\
&= \frac{1}{\sqrt{2\omega}} (\alpha + \alpha^*) = \frac{2}{\sqrt{2\omega}} \Re(\alpha) = \sqrt{\frac{2}{\omega}} \Re(\alpha)
\end{aligned}
$$

And for the variance it follows:

$$
\begin{aligned}
\langle \alpha | \hat{x}^2 | \alpha \rangle =& \frac{1}{2\omega} \langle \alpha | a^2 + a a^\dagger + a^\dagger a + (a^\dagger)^2 | \alpha \rangle \\
=& \frac{1}{2\omega} (\alpha^2 + 2\alpha\alpha^* + 1 + (\alpha^*)^2) \\
=& \frac{1}{2\omega} ((\alpha + \alpha^*)^2 + 1) \\
=& \frac{4}{2\omega} (\Re(\alpha)^2 + 1) \\
(\Delta x)^2 = \langle \alpha | \hat{x}^2 | \alpha \rangle - \langle \alpha | \hat{x} | \alpha \rangle^2 =& \frac{2}{\omega}
\end{aligned}
$$

where it is used that $[a, a^\dagger] = 1$ and $\left\langle \alpha \right| a^\dagger = \alpha^* \left\langle \alpha \right|$.
Analogous considerations can be made for $\hat{p} = -i\sqrt{\frac{\omega}{2}} \left(a - a^\dagger\right)$ to determine Δp, with which it becomes visible that the coherent states are minimum uncertainty states:

$$
\Delta x \Delta p = 1/2
$$

which implies that the coherent states have a gaussian shape with equal width.

The time evolution of $|\alpha\rangle$ is the last missing piece for this analysis:

$$
\begin{aligned}
U(t)\,|\alpha\rangle &= e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \\
&= e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \exp(-iHt)\,|n\rangle \\
&= e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \exp(-iE_n t)\,|n\rangle \\
&= e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i\omega(n+1/2)t}\,|n\rangle \\
&= e^{-\frac{1}{2}|\alpha|^2} e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{(\alpha\cdot e^{-i\omega t})^n}{\sqrt{n!}} |n\rangle\,.
\end{aligned}
$$

The form of the time evolution corresponds to a coherent state with an oscillating α:

$$\alpha(t) = \alpha(t=0)\cdot e^{-i\omega t}$$

Therefore a coherent state stays a coherent state over time, meaning it stays a gaussian with constant width and an oscillating mean position:

$$\langle\hat{x}\rangle = \langle\hat{x}\rangle\,(t=0)\cdot\cos\omega t$$

which can be identified as the displaced gaussians with width $\sigma = 1$ attempted to be described here.
Another, less insightful way to calculate the mean position is using the Ehrenfest theorem:

$$
\begin{aligned}
&\frac{d}{dt}\langle\hat{x}\rangle = -i\,\langle\left[\hat{x},\hat{H}\right]\rangle + \langle\frac{\partial\hat{x}}{\partial t}\rangle = -i\,\langle\left[\hat{x},\frac{1}{2}\hat{p}^2\right]\rangle = -\frac{i}{2}\left(\langle[\hat{x},\hat{p}]\,\hat{p} + \hat{p}\,[\hat{x},\hat{p}]\rangle\right) = \langle\hat{p}\rangle \\
&\frac{d}{dt}\langle\hat{p}\rangle = -i\,\langle\left[\hat{p},\hat{H}\right]\rangle + \langle\frac{\partial\hat{p}}{\partial t}\rangle = -\omega^2\,\langle\hat{x}\rangle \\
&\Rightarrow \langle\hat{x}\rangle = \langle\hat{x}\rangle\,(t=0)\cdot\cos\omega t
\end{aligned}
$$

For examining the variance a different method has to be employed. The fundamental solution of the quantum harmonic oscillator is the Mehler kernel:

$$K(x,y;t) = \frac{1}{\sqrt{2\pi\sinh(2t)}}\exp\Big(-\coth(2t)(x^2+y^2)/2 + \operatorname{csch}(2t)xy\Big)$$

with which the general solution of the Schrödinger equation can be calculated by convolution:

$$\Phi(x,t) = \int dy K(x,y;t)\Phi(y,t=0)$$

The result of this calculation with $\Phi(x,t=0)$ with $x_0 = 0$ and σ arbitrary is taken from "Visual Quantum Mechanics" by Bernd Thaller (1. Ed, 2000) (adjusted to notation):

$$
\begin{aligned}
\psi(x,t) &= \left(\frac{1}{\pi\sigma^2}\right)^{1/4}\left(\cos\omega t + i\frac{1}{\sigma^2}\sin\omega t\right)^{-1/2}\exp\left(-s(t)\frac{x^2}{2}\right) \\
s(t) &= \frac{\frac{1}{\sigma^2}\cos\omega t + i\sin\omega t}{\cos\omega t + i\frac{1}{\sigma^2}\sin\omega t}
\end{aligned}
$$

which describes a gaussian with an oscillating standard deviation.
The mean and variance of the position then follow:

$$
\begin{aligned}
\langle x \rangle = \langle \psi | x | \psi \rangle &= \int_{-\infty}^{\infty} dx \psi * x \psi \\
&= \left(\frac{1}{\pi\sigma^2}\right)^{1/2} \frac{1}{\sqrt{\cos\omega t + i\frac{1}{\sigma^2}\sin\omega t} \cdot \sqrt{\cos\omega t + i\frac{1}{\sigma^2}\sin\omega t}^*} \int_{-\infty}^{\infty} dx \exp\left(-s(t)^* \frac{x^2}{2}\right) x \exp\left(-s(t)\frac{x^2}{2}\right) \\
&= \left(\frac{1}{\pi\sigma^2}\right)^{1/2} \frac{1}{\sqrt{\cos\omega t + i\frac{1}{\sigma^2}\sin\omega t} \cdot \sqrt{\cos\omega t - i\frac{1}{\sigma^2}\sin\omega t}} \int_{-\infty}^{\infty} dx \exp\left(-\Re(s(t))x^2\right) x = 0
\end{aligned}
$$

$$
\begin{aligned}
\langle x^2 \rangle = \langle \psi | x^2 | \psi \rangle &= \int_{-\infty}^{\infty} dx \psi^* x^2 \psi \\
&= \left(\frac{1}{\pi\sigma^2}\right)^{1/2} \frac{1}{\sqrt{\cos^2\omega t + \frac{1}{\sigma^4}\sin^2\omega t}} \int_{-\infty}^{\infty} dx \exp\left(-\Re(s(t))x^2\right) x^2 \\
&= \left(\frac{1}{\pi\sigma^2}\right)^{1/2} \frac{1}{\sqrt{\cos^2\omega t + \frac{1}{\sigma^4}\sin^2\omega t}} \frac{\sqrt{\pi}}{2\Re(s(t))^{3/2}} \\
&= \frac{\sqrt{\pi}}{2}\left(\frac{1}{\pi\sigma^2}\right)^{1/2} \frac{1}{\sqrt{\cos^2\omega t + \frac{1}{\sigma^4}\sin^2\omega t}} \left(\cos^2\omega t + \frac{1}{\sigma^4}\sin^2\omega t\right)^{3/2} \sigma^3 \\
&= \frac{\sigma^2}{2}\left(\cos^2\omega t + \frac{1}{\sigma^4}\sin^2\omega t\right) \\
&= \frac{\sigma^2}{2}\frac{1}{2}\left(1 + \cos(2\omega t) + \frac{1}{\sigma^4} - \frac{1}{\sigma^4}\cos(2\omega t)\right) \\
&= \frac{\sigma^2}{4}\left(1 + \frac{1}{\sigma^4} + \cos(2\omega t)\left(1 - \frac{1}{\sigma^4}\right)\right) \\
\Rightarrow (\Delta x)^2 &= \frac{\sigma^2}{4}\left(1 + \frac{1}{\sigma^4} + \cos(2\omega t)\left(1 - \frac{1}{\sigma^4}\right)\right) \\
&= \left(\frac{\sigma^2}{4} + \frac{1}{4\sigma^2}\right) + \cos(2\omega t)\left(\frac{\sigma^2}{4} - \frac{1}{4\sigma^2}\right)
\end{aligned}
$$

using:

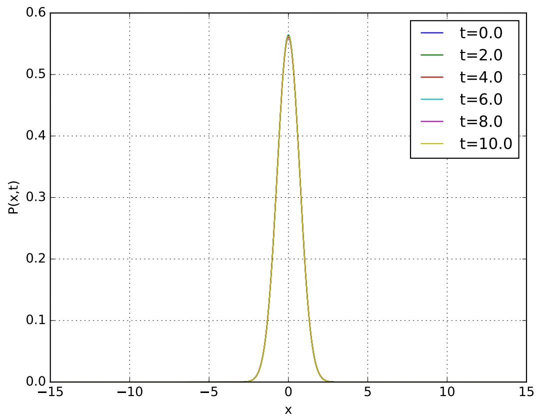
$$
\begin{aligned}
\Re(s(t)) &= \Re\left(\frac{\frac{1}{\sigma^2}\cos\omega t + i\sin\omega t}{\cos\omega t + i\frac{1}{\sigma^2}\sin\omega t} \cdot \frac{\cos\omega t - i\frac{1}{\sigma^2}\sin\omega t}{\cos\omega t - i\frac{1}{\sigma^2}\sin\omega t}\right) \\
&= \frac{\frac{1}{\sigma^2}\cos^2\omega t + \frac{1}{\sigma^2}\sin^2\omega t}{\cos^2\omega t + \frac{1}{\sigma^4}\sin^2\omega t} = \frac{\frac{1}{\sigma^2}}{\cos^2\omega t + \frac{1}{\sigma^4}\sin^2\omega t}
\end{aligned}
$$

Simulation method

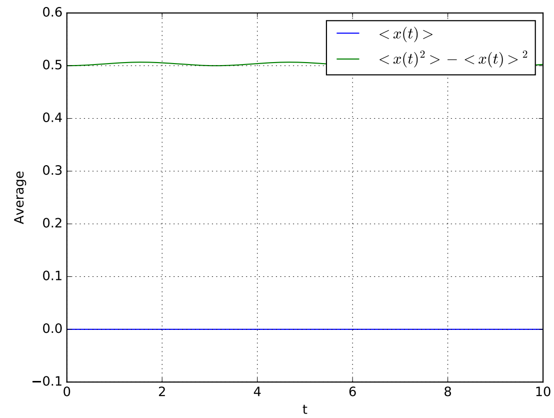
The simulation method is identical to the method used and outlines in exercise 6, though parameters have been modified. For reference the model is explained once more in the appendix on page 8.

Simulation results

Plots of simulation runs with different parameter tuples ω, σ, x_0 can be found in the figures 1, 2, 3, 4 and 5.

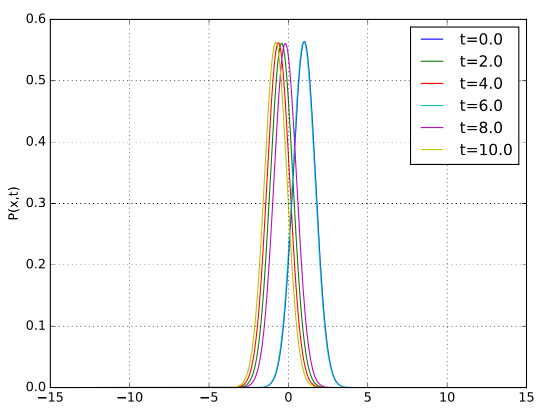


(a) Probability distribution of the wave function at different times t.

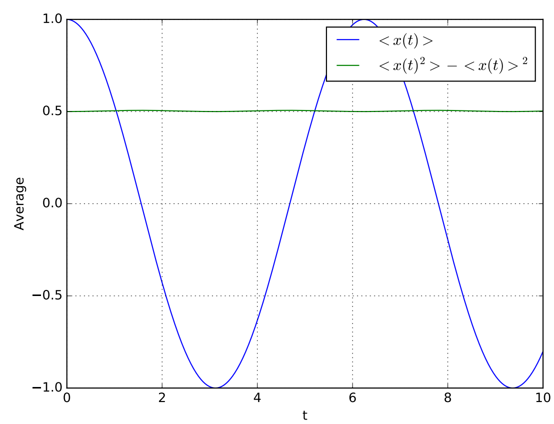


(b) Mean (blue) and variance (green) of the position operator over time.

Figure 1: Simulation results for $\omega = 1$, $\sigma = 1$, $x_0 = 0$.

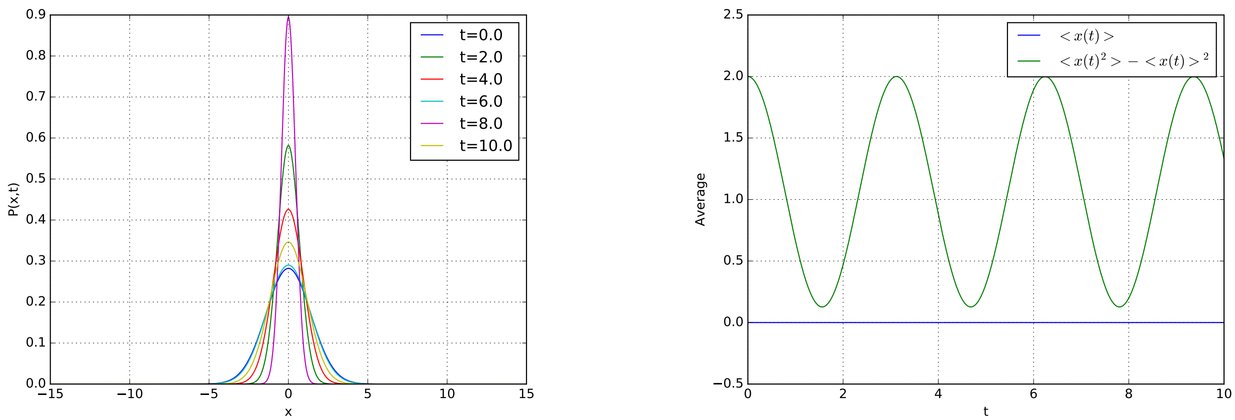


(a) Probability distribution of the wave function at different times t.



(b) Mean (blue) and variance (green) of the position operator over time.

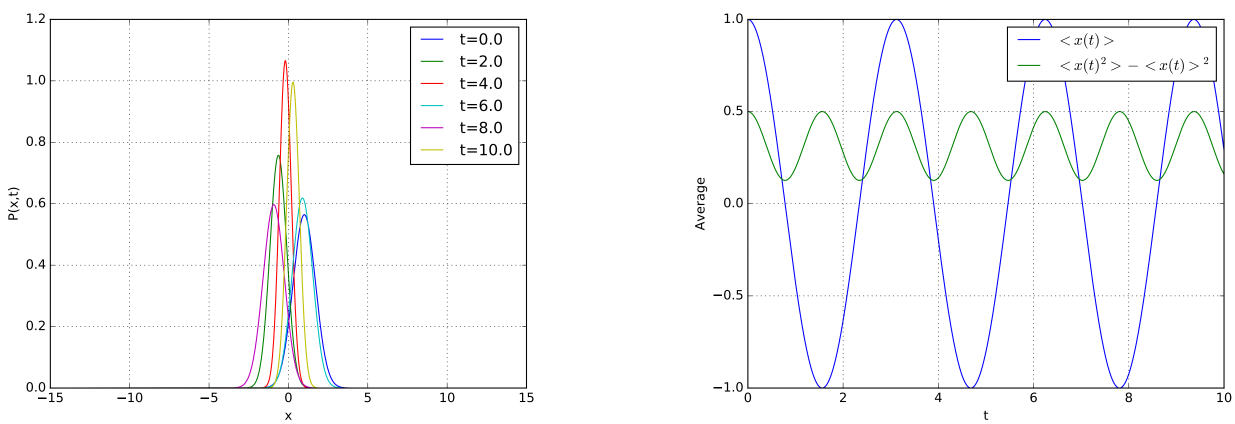
Figure 2: Simulation results for $\omega = 1$, $\sigma = 1$, $x_0 = 1$.



(a) Probability distribution of the wave function at different times t.

(b) Mean (blue) and variance (green) of the position operator over time.

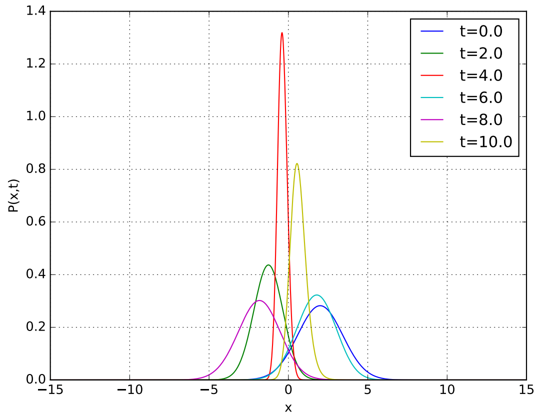
Figure 3: Simulation results for $\omega = 1$, $\sigma = 2$, $x_0 = 0$.



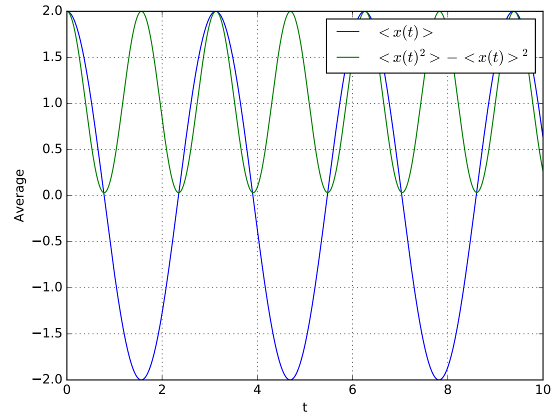
(a) Probability distribution of the wave function at different times t.

(b) Mean (blue) and variance (green) of the position operator over time.

Figure 4: Simulation results for $\omega = 2$, $\sigma = 1$, $x_0 = 1$.



(a) Probability distribution of the wave function at different times t.



(b) Mean (blue) and variance (green) of the position operator over time.

Figure 5: Simulation results for $\omega = 2$, $\sigma = 2$, $x_0 = 2$.

Discussion

The simulation gives plausible results that match our analytical prediction. The system with $\omega = 1$, $\sigma = 1$, $x_0 = 0$ is stationary, as expected, since it is the ground state $|0\rangle$ of the quantum harmonic oscillator. It is also a coherent state with $\alpha = 0$, which implies that there is no oscillation too, since $\alpha = 0 \Rightarrow \Re(\alpha) = 0$. A sinusodial oscillation in the mean position with frequency ω/π can be observed for $x_0 \neq 0$. With $\sigma = 1$ these states correspond to coherent states, which are minimally uncertain. This makes them the “most classical” state that can be constructed, so it is plausible to observe the classical limit of a particle oscillating in the potential unchanged here, which is the case. This also motivates the coherent states sometimes being called “quasi-classical” states.

An also sinusodial oscillation of the width of the gaussian can be observed with the expected frequency $2\omega/\pi$. For $\omega = 1$, $\sigma = 2$, $x_0 = 1$ the functional dependence of that oscillation matches the prediction exactly.

The frequencies of the oscillations of both variance and mean position holds true even for the cases of both $x_0 \neq 0$ and $\sigma \neq 1$, which could not be handled analytically in full.

In conclusion the formula approach was successfully used to simulate the dynamics of the quantum harmonic oscillator. As stated in the previous exercise, the approach is simple and effective, but can not trivially be extended to higher dimensions and requires a fair amount computational investment to avoid numerical errors, which are easily introduced if the time step is chosen too large.

Appendix

Simulation model

Using finite differences the spatial derivative in the Schrödinger equation becomes:

$$\frac{\partial^2}{\partial x^2}\Psi(x,t) = \frac{\Psi(x+\Delta,t) - 2\Psi(x,t) + \Psi(x-\Delta,t)}{\Delta^2}$$

with $\Delta = 0.025$ being the spacing of our simulation grid.
The Schrödinger equation in one dimension then becomes

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi(x,t) &= -\frac{\Psi(x+\Delta,t) - 2\Psi(x,t) + \Psi(x-\Delta,t)}{2\Delta^2} + V(x)\Psi(x,t) \\ &= \frac{1}{\Delta^2}\left(-\frac{1}{2}\Psi(x+\Delta,t) - \frac{1}{2}\Psi(x-\Delta,t) + \left(1+\Delta^2 V(x)\right)\Psi(x,t)\right). \end{aligned}$$

Our discretized Hamiltonian can then be read as:

$$i\frac{\partial}{\partial t}\begin{pmatrix}\Psi_1(t)\\ \Psi_2(t)\\ \Psi_3(t)\\ \vdots\\ \vdots\\ \Psi_L(t)\end{pmatrix} = \underbrace{\frac{1}{\Delta^2}\begin{pmatrix} 1+\Delta^2 V_1 & -1/2 & 0 & & 0 \\ -1/2 & 1+\Delta^2 V_2 & -1/2 & 0 & 0 \\ 0 & -1/2 & 1+\Delta^2 V_3 & & \\ & & & \ddots & 0 \\ & & & & -1/2 \\ 0 & & & 0 \quad -1/2 & 1+\Delta^2 V_L \end{pmatrix}}_{H}\begin{pmatrix}\Psi_1(t)\\ \Psi_2(t)\\ \Psi_3(t)\\ \vdots\\ \vdots\\ \Psi_L(t)\end{pmatrix}$$

with $V_i = V(i\Delta)$, $\Psi_i(t) = \Psi(x = i\Delta, t)$ and $L = 1201$ being the size of our simulation grid (in number of grid points).
The Hamiltonian can then be decomposed into a sum:

$$\begin{aligned} H = V + K_1 + K_2 = \frac{1}{\Delta^2}&\begin{pmatrix} 1+\Delta^2 V_1 & 0 & 0 & & & 0 \\ 0 & 1+\Delta^2 V_2 & 0 & 0 & & 0 \\ 0 & 0 & 1+\Delta^2 V_3 & & & \\ & & & \ddots & & 0 \\ & & & & 1+\Delta^2 V_{L-1} & 0 \\ 0 & & & 0 & 0 & 1+\Delta^2 V_L \end{pmatrix} \\ + \frac{1}{\Delta^2}\begin{pmatrix} 0 & -1/2 & 0 & & & 0 \\ -1/2 & 0 & 0 & & & \\ 0 & 0 & 0 & & & \\ & & \ddots & -1/2 & 0 \\ & & -1/2 & 0 & 0 \\ 0 & & 0 & 0 & 0 \end{pmatrix} &+ \frac{1}{\Delta^2}\begin{pmatrix} 0 & 0 & 0 & & & 0 \\ 0 & 0 & -1/2 & & & \\ 0 & -1/2 & 0 & & & \\ & & & \ddots & & 0 \\ & & & & 0 & -1/2 \\ 0 & & & 0 & -1/2 & 0 \end{pmatrix} \end{aligned}$$

The time evolution operator can then be written as:

$$U(\tau) = e^{-i\tau H} \approx e^{-i\tau K_1/2} e^{-i\tau K_2/2} e^{-i\tau V} e^{-i\tau K_2/2} e^{-i\tau K_1/2}$$

where $\tau = 0.00025$ is the time step of our simulation.

The full expressions are the following:

$$
e^{-i\tau K_1/2} = \begin{pmatrix}
c & is & & & & & & \dots & 0 \\
is & c & 0 & & & & & & \vdots \\
 & 0 & c & is & & & & & \\
 & & is & c & 0 & & & & \\
 & & & 0 & c & is & & & \\
 & & & & is & c & 0 & & \\
 & & & & & 0 & \ddots & is & \\
\vdots & & & & & & is & \ddots & 0 \\
0 & \dots & & & & & & 0 & 1
\end{pmatrix}
$$

$$
e^{-i\tau K_2/2} = \begin{pmatrix}
1 & 0 & & & & & & \dots & 0 \\
0 & c & is & & & & & & \vdots \\
 & is & c & 0 & & & & & \\
 & & 0 & c & is & & & & \\
 & & & is & c & 0 & & & \\
 & & & & 0 & c & is & & \\
 & & & & & is & \ddots & 0 & \\
\vdots & & & & & & 0 & \ddots & is \\
0 & \dots & & & & & & is & c
\end{pmatrix}
$$

$$
e^{-i\tau V} = \frac{1}{\Delta^2} \begin{pmatrix}
1+\Delta^2 V_1 & 0 & 0 & & & 0 \\
0 & 1+\Delta^2 V_2 & 0 & 0 & & 0 \\
0 & 0 & 1+\Delta^2 V_3 & & & \\
 & & & \ddots & & 0 \\
 & & & & 1+\Delta^2 V_{L-1} & 0 \\
0 & & & 0 & 0 & 1+\Delta^2 V_L
\end{pmatrix}
$$

where $c = \cos\left(\tau/(4\Delta^2)\right)$ and $s = \sin\left(\tau/(4\Delta^2)\right)$.
In each timestep a set of complex values for each grid point is then updated using the time evolution operator.

Shared constants (conf.py)

```
Delta = 0.025
tau = 0.00025
m = 40000
xMin, xMax = -15, 15
xRange = xMax - xMin
L = (xRange / Delta) + 1
assert abs(L - int(L)) < 1e-8
L = int(L)
```

Simulation script

```
import math
import cmath
import sys
import numpy as np
import matplotlib.pyplot as plt

from conf import *

```

```
def sim(Omega, sigma, x0):
    def V(x):
        return Omega*Omega / 2 * x*x

    def psi_t0(x):
        ret = math.pow(math.pi * sigma*sigma, -0.25)
        ret *= math.exp(-(x-x0)*(x-x0)/(2*sigma*sigma))
        return ret

    psi = np.zeros(L, dtype=complex)
    for l in range(L):
        psi[l] = psi_t0(xMin + l*Delta)

    expV = np.zeros((L,L), dtype=complex)
    for l in range(L):
        expV[l][l] = cmath.exp(-1j * tau * (1/(Delta*Delta) + V(xMin + l*Delta)
        ))

    c = math.cos(tau / (4*Delta*Delta))
    s = math.sin(tau / (4*Delta*Delta))

    expK1 = np.eye(L, dtype=complex) * c
    expK1[L-1][L-1] = 1
    expK2 = np.eye(L, dtype=complex) * c
    expK2[1][1] = 1

    for l in range(L):
        if l+1 < L:
            if l % 2 == 0:
                expK1[l+1][l] = expK1[l][l+1] = 1j * s
            else:
                expK2[l+1][l] = expK2[l][l+1] = 1j * s

    U = expK1 @ expK2 @ expV @ expK2 @ expK1

    out = np.zeros((m+1, L), dtype=complex)

    for i in range(m+1):
        if math.floor(i/m*100) != math.floor((i-1)/m*100):
            print(math.floor(i/m*100), "%")
        t = i * tau

        psi = np.dot(U, psi)
        out[i] = psi

    return out

# on sheet: (1,1,0), (1,1,1), (1,2,0), (2,1,1), (2,2,2)
Omega, sigma, x0 = int(sys.argv[1]), int(sys.argv[2]), int(sys.argv[3])
set_name = "Omega={}, sigma={}, x0={}".format(Omega, sigma, x0)
print(set_name)
data = sim(Omega, sigma, x0)
np.save(set_name, data)
```

Plot script

```python
import os
import sys
import numpy as np
import matplotlib.pyplot as plt

from conf import *
x = np.arange(L) * Delta + xMin

def pd(psi):
    v = np.absolute(psi)
    return v*v

def expect(psi, f):
    assert f.shape == psi.shape
    return np.dot(f, pd(psi)) * Delta

def mean_pos(psi):
    return expect(psi, x)

def var_pos(psi):
    mp = mean_pos(psi)
    return expect(psi, x*x) - mp*mp

data = np.load(sys.argv[1])
name = sys.argv[1][:-4]

t = np.arange(m+1) * tau
mean = np.zeros(m+1)
var = np.zeros(m+1)
for i in range(m+1):
    psi = data[i]
    # snapshots at t=0,2,4,6,8,10
    # => i = 0, 8000, 16000, ..., 40000
    if i % 8000 == 0:
         plt.plot(x, pd(psi), label="t={}".format(i * tau))

    mean[i] = mean_pos(psi)
    var[i] = var_pos(psi)

plt.xlabel("x")
plt.ylabel("P(x,t)")
plt.grid(True)
plt.legend()
plt.savefig(name + "-probdist.pdf")
plt.show()
plt.close()

plt.xlabel("t")
plt.ylabel("Average")
plt.grid(True)
plt.plot(t, mean, label="$<x(t)>$")
plt.plot(t, var, label="$<x(t)^2> - <x(t)>^2$")
plt.legend()
plt.savefig(name + "-pos.pdf")
plt.show()
```