Exam: A product formula approach to solve the Schrödinger equation for harmonic potentials

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Introduction

In this exercise, I solve the time-dependent Schrödinger equation for initially coherent and squeezed states in a one-dimensional harmonic potential. First, the numerical simulation method is derived from the Schrödinger equation, after which analytical expectations for different model parameters are discussed. These expectations are subsequently compared to the produced simulation results and interpreted. Finally, I summarize the findings and give a listing of the simulation program. I will denote matrices by uppercase latin characters O, operators by uppercase latin characters with hats $\hat{O}$ and vectors, ket-vectors, functions, scalars etc. as usual throughout the text.

Simulation model and method

In quantum theory, states of a system with Hamiltonian $\hat{H}$ evolve according to the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle. \tag{1}$$

For a harmonic time-independent, one-dimensional potential $V(x) = \Omega^2 m x^2/2$, Eq. 1 in position representation reads

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

Choosing dimensionless variables, s.t. $\hbar = m = 1$ and discretizing Eq. 2 centrally in space for a small space step Δ one obtains

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{\psi(x+\Delta,t) - 2\psi(x,t) + \psi(x-\Delta,t)}{2\Delta^2} + \frac{\Omega^2}{2}x^2\psi(x,t) \tag{3}$$

$$= -\frac{\psi(x+\Delta,t) + \psi(x-\Delta,t)}{2\Delta^2} + \big(\frac{1}{\Delta^2} + \frac{\Omega^2}{2}x^2\big)\psi(x,t). \tag{4}$$

By the discretization of space we must rewrite $x \to j_k\Delta$. Then $\psi(x,t)$ can be written as a vector with components defined at discrete space positions $j_k\Delta$, i.e. $\psi_{j_k}(t) = \psi(j_k\Delta,t)$ for integers j_k indexed by $k = 1,2,...,L$. This notation allows to offset the origin of space $j_0\Delta$ to any point in discretized space. Thus, Eq. 4 can be written in matrix form:

$$i\frac{\partial}{\partial t}\begin{bmatrix}\psi_{j_1}(t)\\ \psi_{j_2}(t)\\ \psi_{j_3}(t)\\ \vdots\\ \psi_{j_{L-1}}(t)\\ \psi_{j_L}(t)\end{bmatrix} = \underbrace{\frac{1}{\Delta^2}\begin{bmatrix}1+\Delta^4 j_1^2\Omega^2/2 & -1/2 & 0 & & & 0\\ -1/2 & 1+\Delta^4 j_2^2\Omega^2/2 & -1/2 & & & \\ 0 & -1/2 & 1+\Delta^4 j_3^2\Omega^2/2 & & & \\ & & & \ddots & & 0\\ & & & & 1+\Delta^4 j_{L-1}^2\Omega^2/2 & -1/2\\ 0 & & & 0 & -1/2 & 1+\Delta^4 j_L^2\Omega^2/2\end{bmatrix}}_{H}\underbrace{\begin{bmatrix}\psi_{j_1}(t)\\ \psi_{j_2}(t)\\ \psi_{j_3}(t)\\ \vdots\\ \psi_{j_{L-1}}(t)\\ \psi_{j_L}(t)\end{bmatrix}}_{\vec{\psi}(t)}. \tag{5}$$

Note that H is a real Hermitian matrix. Eq. 5 is a standard first-order matrix differential equation with general solution

$$\vec{\psi}(t) = e^{-itH}\vec{\psi}(t=0) = U\vec{\psi}(t=0). \tag{6}$$

The matrix U thus evolves $\vec{\psi}$ in time. As H is Hermitian, U is unitary and hence its action leaves the norm of $\vec{\psi}$ invariant, which coincides with the conservation of probability at each point in time during the evolution. The special structure of H further allows to decompose it into the sum of one diagonal matrix V and two (mostly) block-diagonal matrices K_1 and K_2:

$$H = V + K_1 + K_2 = \frac{1}{\Delta^2}\begin{bmatrix} 1+\Delta^4 j_1^2\Omega^2/2 & 0 & 0 & & & 0 \\ 0 & 1+\Delta^4 j_2^2\Omega^2/2 & 0 & & & \\ 0 & 0 & 1+\Delta^4 j_3^2\Omega^2/2 & & & \\ & & & \ddots & & 0 \\ & & & & 1+\Delta^4 j_{L-1}^2\Omega^2/2 & 0 \\ 0 & & & 0 & 0 & 1+\Delta^4 j_L^2\Omega^2/2 \end{bmatrix} + \\ + \frac{1}{\Delta^2}\begin{bmatrix} 0 & -1/2 & 0 & & & 0 \\ -1/2 & 0 & 0 & & & \\ 0 & 0 & 0 & & & \\ & & & \ddots & -1/2 & 0 \\ & & & -1/2 & 0 & 0 \\ 0 & & & 0 & 0 & 0 \end{bmatrix} + \frac{1}{\Delta^2}\begin{bmatrix} 0 & 0 & 0 & & & 0 \\ 0 & 0 & -1/2 & & & \\ 0 & -1/2 & 0 & & & \\ & & & \ddots & & 0 \\ & & & & 0 & -1/2 \\ 0 & & & 0 & -1/2 & 0 \end{bmatrix}. \tag{7}$$

Now, the Suzuki-Trotter product formula can be employed to approximate

$$e^{-itH} = e^{-it(V+K_1+K_2)} \approx e^{-itK_1/2}e^{-itK_2/2}e^{-itV}e^{-itK_2/2}e^{-itK_1/2}, \tag{8}$$

which is subsequently trotterized to

$$e^{-itK_1/2}e^{-itK_2/2}e^{-itV}e^{-itK_2/2}e^{-itK_1/2} \approx \left(e^{-i\tau K_1/2}e^{-i\tau K_2/2}e^{-i\tau V}e^{-i\tau K_2/2}e^{-i\tau K_1/2}\right)^m \tag{9}$$

with time-step $\tau = t/m$ for large Trotter number m. When one computes the matrix exponentials of the blocks in K_1 and K_2 by expanding into exponential series one obtains

$$e^{i\alpha X} = \begin{bmatrix} \cos(\alpha) & i\sin(\alpha) \\ i\sin(\alpha) & \cos(\alpha) \end{bmatrix}, \tag{10}$$

for σ_x-Pauli matrix X and $\alpha = \tau/4\Delta^2$. For the 0 in the first (last) position of the block-diagonal matrices one obtains the exponential $e^0 = 1$. Thus, to evolve a given initial state $\vec{\psi}(t=0)$ for a time $t = m\tau$ the sequence in the brackets of Eq. 9 is applied m times to $\vec{\psi}(t=0)$, which becomes more accurate for larger m (and correspondingly smaller τ). For the matrix exponentials of K_i, Eq. 10 is applied pairwise to corresponding pairs in $\vec{\psi}$, while the matrix exponential of V can be stored in a column vector (due to diagonality) and multiplied directly element-wise with the previously transformed $\vec{\psi}$.

Analytical expectations

In order to calculate expectation values and other moments it is beneficial to take a step back and to consider the Hamiltonian from Eq. 2 in operator representation, where $x \to \hat{x}$ and $-i\partial_x \to \hat{p}$, thus

$$\hat{H} = \frac{1}{2}(\hat{p}^2 + \Omega^2\hat{x}^2). \tag{11}$$

The Hamiltonian can be factored by defining $\hat{x} = (\hat{a} + \hat{a}^\dagger)/\sqrt{2\Omega}$ and $\hat{p} = -i\sqrt{\Omega/2}(\hat{a} - \hat{a}^\dagger)$, where we call $\hat{a}$ the *annihilation* operator and $\hat{a}^\dagger$ the *creation* operator which are correspondingly $\hat{a} = (\Omega\hat{x} + i\hat{p})/\sqrt{2\Omega}$ and $\hat{a}^\dagger = (\hat{a})^\dagger$, such that $[\hat{a}, \hat{a}^\dagger] = I$ where I is the identity matrix. Substituting $\hat{p}$ and $\hat{x}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$ into Eq. 11 leads to

$$\hat{H} = \frac{\Omega}{4}(2\hat{a}\hat{a}^\dagger + 2\hat{a}^\dagger\hat{a} - \hat{a}^2 + \hat{a}^2 - (\hat{a}^\dagger)^2 + (\hat{a}^\dagger)^2) = \Omega(\hat{a}^\dagger\hat{a} + \frac{I}{2}). \tag{12}$$

Now, we consider the Heisenberg picture. In this picture the time-dependence is carried by the operators instead of the states. We note that for $\hat{x}$ the time-dependence is completely carried by its constituent operators $\hat{a}$ and $\hat{a}^\dagger$, i.e. $\hat{x}(t) = (\hat{a}(t) + \hat{a}^\dagger(t)/\sqrt{2\Omega}$. Thus, to find $\hat{x}(t)$ we have to find $\hat{a}(t)$ and $\hat{a}^\dagger(t)$. Using the Heisenberg equation of motion for the (time-independent) Hamiltonian and making use of $[\hat{O}, I] = [\hat{O}(t), \hat{O}(t)] = 0$ for a generic operator $\hat{O}$ we obtain

$$\frac{\partial}{\partial t}\hat{a}(t) = i[\hat{H}, \hat{a}(t)] = i\Omega[\hat{a}^\dagger(t)\hat{a}(t) + I/2, \hat{a}(t)] = -i\Omega\hat{a}(t). \tag{13}$$

The result is a first-order differential matrix equation which has general solution $\hat{a}(t) = \hat{A}e^{-i\Omega t}$, where $\hat{A}$ is determined via the initial condition $\hat{a}(0) = \hat{A} \equiv \hat{a}$. Subsequently taking the Hermitian conjugate yields $\hat{a}^\dagger(t) = \hat{a}^\dagger e^{i\Omega t}$. Thus, an expression for the time-dependent position operator has been found

$$\hat{x}(t) = (\hat{a}e^{-i\Omega t} + \hat{a}^\dagger e^{i\Omega t})/\sqrt{2\Omega} = \hat{x}(e^{-i\Omega t} + e^{i\Omega t}) + \frac{i\hat{p}}{\Omega}(e^{-i\Omega t} - e^{i\Omega t}) = \hat{x}\cos(\Omega t) + \frac{\hat{p}}{\Omega}\sin(\Omega t). \tag{14}$$

Further, using the equivalence between Heisenberg and Schrödinger picture and inserting the completeness relation $\int_{-\infty}^{+\infty} dx|x\rangle\langle x| = I$, the expectation value of the time-dependent position operator can be determined as

$$\langle\hat{x}(t)\rangle = \langle\psi(t)|\hat{x}|\psi(t)\rangle = \langle\psi(0)|\hat{x}(t)|\psi(0)\rangle = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dxdx' \underbrace{\langle\psi(0)|x\rangle}_{\psi^*(x)} \underbrace{\langle x|\hat{x}(t)|x'\rangle}_{\delta(x-x')x(t)} \underbrace{\langle x'|\psi(0)\rangle}_{\psi(x')}. \tag{15}$$

Substituting the initial (real) wave function and the time-dependent position operator from Eq. 14 in position representation,

$$\psi(x) = \psi^*(x) = \frac{1}{\pi^{1/4}\sqrt{\sigma}}e^{-(x-x_0)^2/2\sigma^2}, \tag{16}$$

$$x(t) = x\cos(\Omega t) - \frac{i\sin(\Omega t)}{\Omega}\frac{\partial}{\partial x}, \tag{17}$$

into Eq. 15 together with setting $x_0 = 0$ yields

$$\langle x(t)\rangle = \frac{1}{\sqrt{\pi}\sigma}\int_{-\infty}^{+\infty} dx\big(\cos(\Omega t) + \frac{i\sin(\Omega t)}{\Omega\sigma^2}\big)\underbrace{x}_{\text{odd}}\underbrace{e^{-x^2/2\sigma^2}}_{\text{even}} = 0. \tag{18}$$

So, the expectation value for $x_0 = 0$ is 0 for all time, no matter which values for σ or Ω are chosen. This is a similar result as for a classical harmonic oscillator: Without displacement no movement. The only difference between classical and quantum is that for the former x and p change directly, while for the latter it is the expectation value of the probability distribution over x and p which changes with time. One can show that in the classical limit (at a certain time/length/mass scale) the distributions converge towards delta functions with well defined expectation values. In this case, the quantum system essentially behaves like a classical one. For the special case of Eq. 15, we see a probability distribution over x (quantum) for which the expectation value is well-defined (classical) at all times. Next, we are going to calculate the second moment of the time-dependent position operator by again making use of the completeness of the position basis to convert states and operators into position representation:

$$\begin{aligned}
\langle\big(x(t)\big)^2\rangle &= \langle\psi(0)|\big(\cos^2(\Omega t)\hat{x}^2 + \frac{\sin^2(\Omega t)}{\Omega^2}\hat{p}^2 + \frac{\cos(\Omega t)\sin(\Omega t)}{\Omega}(\hat{x}\hat{p} + \hat{p}\hat{x})\big)|\psi(0)\rangle \\
&= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dxdx'dx''\langle\psi(0)|x\rangle\langle x|\big(\cos^2(\Omega t)\hat{x}|x'\rangle\langle x'|\hat{x}+ \\
&+ \frac{\sin^2(\Omega t)}{\Omega^2}\hat{p}|x'\rangle\langle x'|\hat{p} + \frac{\cos(\Omega t)\sin(\Omega t)}{\Omega}(\hat{x}|x'\rangle\langle x'|\hat{p} + \hat{p}|x'\rangle\langle x'|\hat{x})\big)|x''\rangle\langle x''|\psi(0)\rangle \\
&= \int_{-\infty}^{+\infty} dx\big(\underbrace{\cos^2(\Omega t)x^2\psi^2(x)}_{\equiv I_1} \underbrace{-\frac{\sin^2(\Omega t)}{\Omega^2}\psi(x)\frac{\partial^2}{\partial x^2}\psi(x)}_{\equiv I_2} \underbrace{-\frac{i\cos(\Omega t)\sin(\Omega t)}{\Omega}\psi(x)\big(x\frac{\partial}{\partial x} + \frac{\partial}{\partial x}x\big)\psi(x)}_{\equiv I_3}\big).
\end{aligned} \tag{19}$$

The three above integrals can be solved by using two Gauss integral identities $\int_{-\infty}^{+\infty} e^{-x^2/\sigma^2} = \sqrt{\pi}\sigma$ and $\int_{-\infty}^{+\infty} x^2 e^{-x^2/\sigma^2} = \sqrt{\pi}\sigma^3/2$ and by calculating the derivatives $\partial_x\psi(x) = -\psi(x)x/\sigma$, $\partial_{xx}\psi(x) = (x^2/\sigma^4 - 1/\sigma^2)\psi(x)$ and $\partial_x\psi(x)x = (1 - x^2/\sigma^2)\psi(x)$ after which one obtains

$$\int_{-\infty}^{+\infty} I_1 dx = \frac{\sigma^2}{2}\cos^2(\Omega t), \qquad \int_{-\infty}^{+\infty} I_2 dx = \frac{1}{2\Omega^2\sigma^2}\sin^2(\Omega t), \qquad \int_{-\infty}^{+\infty} I_3 dx = 0 \tag{20}$$

Thus, the second moment and, as $\langle x(t)\rangle = 0$, also the variance is found to be

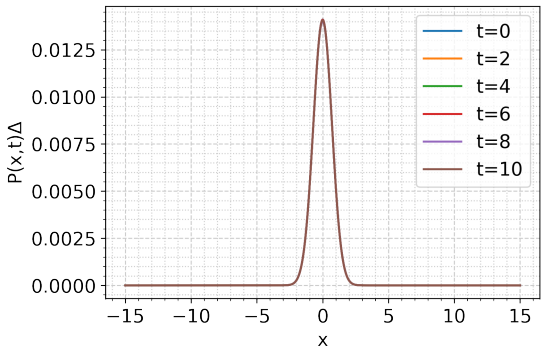
$$\big(\Delta x(t)\big)^2 = \langle\big(x(t)\big)^2\rangle - \langle x(t)\rangle^2 = \frac{\sigma^2}{2}\cos^2(\Omega t) + \frac{1}{2\Omega^2\sigma^2}\sin^2(\Omega t). \tag{21}$$

We note that for $\sigma = \Omega = 1$ the variance is $\big(\Delta x(t)\big)^2 = (\cos^2(t) + \sin^2(t))/2 = const. = 1/2$. One can do the same calculation in momentum representation and would obtain $\big(\Delta p(t)\big)^2 = const. = 1/2$. Thus the uncertainty product is at a minimum of

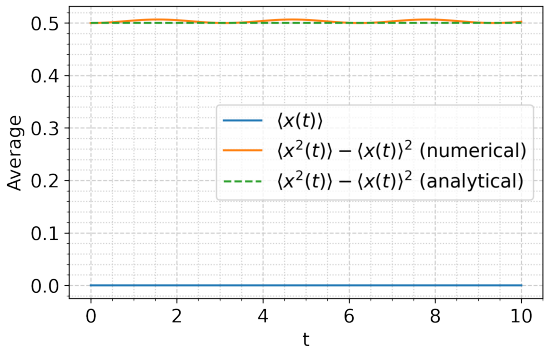
$\Delta x(t)\Delta p(t) = const. = 1/2$. We recognize $\psi(x)$ as the ground state wave function of the Hamiltonian with the vacuum energy $1/2$. Furthermore, if we translate this state $x_0 \neq 0$ we create by definition a *coherent* state, which also shows a minimum in its Heisenberg uncertainty product. Furthermore, when we change spread σ of the initial Gaussian wave function we produce a *squeezed* state which is momentum(p)-squeezed (i.e. larger uncertainty in position or *anti*-squeezed in position) for $\sigma > 1$ and position(x)-squeezed for $0 < \sigma < 1$. Similar to coherent states, squeezed states also fulfill the minimum uncertainty product at all times. However, as we can see from Eq. 21, an initial squeezing causes an oscillating variance in position (and momentum) space during the evolution, such that at certain times the variance in one of these so-called *quadratures* can reach even lower values than $1/2$ (at the expense of larger uncertainty in the other quadrature at the same time). Lastly, varying Ω changes the frequency and thereby also the energy scale of the quantum harmonic oscillator. From Eq. 21 we can further see that not only the oscillation frequency of the variance changes but also that the amplitude of the sine-term is quadratically surpressed causing it to vanish for large Ω. In this case the variance comes closer and closer to 0 at certain times which is particularly useful for certain applications in which one wants to determine the position (or momentum) of a particle with very high precision, as in interferometry.

Simulation results

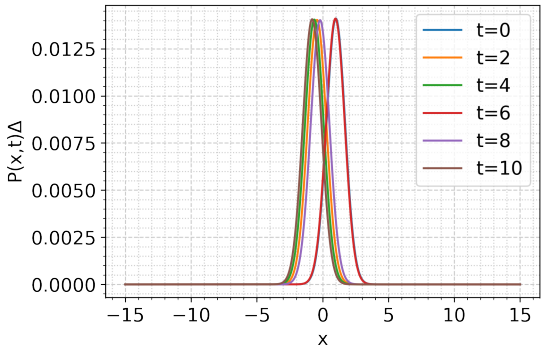
What was explained from an analytical standpoint in the previous paragraph was also obtained from numerical simulation. In Fig. 1 one can see the time evolution of a coherent state, i.e. for $\Omega = \sigma = 1$. In both cases of Figs. 1a–1b and 1c–1d the variance remains constantly $1/2$ throughout the time evolution. Only in the second case where $x_0 = 1$ we see an oscillation of $\langle x(t)\rangle$. Here, the expectation value of the quantum oscillator changes between x_0 and $-x_0$. This is similar to a classical oscillator with $x_0 = 1$. We can further notice that the shape of the probability distribution is not changing, i.e. it remains *coherent* at all times - another property which we also see in the classical oscillator. For these reasons *coherent* states are considered the most *classical* of the the quantum states. In Fig. 1b we see a small deviation between analytical and numerical results. This vanishes when we choose a more refined time resolution.



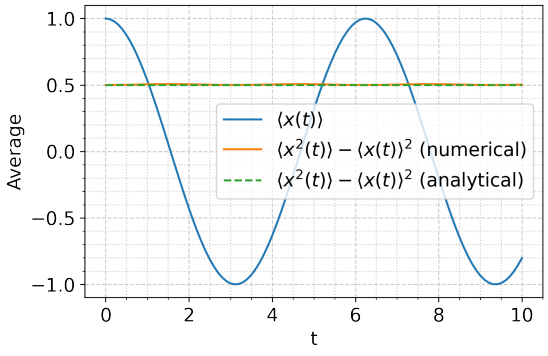
(a) Probability in space for $(\Omega, \sigma, x_0) = (1,1,0)$



(b) Mean and variance in time for $(\Omega, \sigma, x_0) = (1,1,0)$



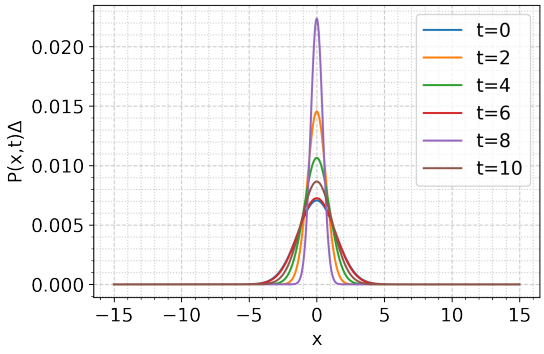
(c) Probability in space for $(\Omega, \sigma, x_0) = (1,1,1)$



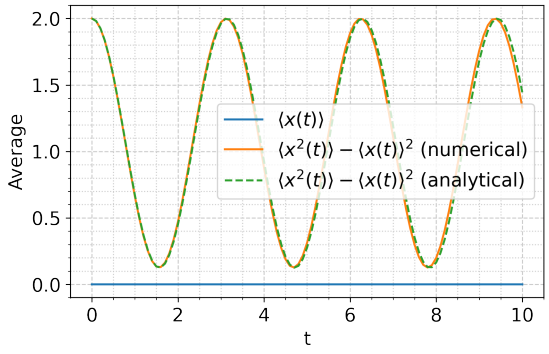
(d) Mean and variance in time for $(\Omega, \sigma, x_0) = (1,1,1)$

Figure 1. Time evolution of a coherent state with (**a**,**b**) and without (**c**,**d**) displacement. In both cases the variance remains $1/2$ at all times while for non-zero displacement the entire probability function oscillates in space.

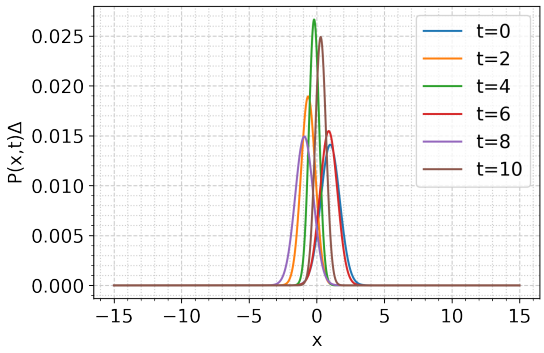
As previously discussed if one chooses $\sigma > 1$, one obtains a momentum-squeezed state, i.e. a state that starts with larger initial variance in position and then oscillates with a period of $2\pi/\Omega$ between $\sigma^2/2$ at $n\pi/2$ for even $n \geq 0$ and $1/(2\Omega^2\sigma^2)$ at $m\pi/2$ for odd $m \geq 1$. As the uncertainty product must be at a minimum $1/2$ at all times we must have a very similar but opposing oscillation (with same frequency) in momentum space. If displacement is added, as in Fig. 2f, the mean additionally oscillates similar to the case of coherent states without any change to the variance. One can note that for example in Fig. 2b, the error for the numerically obtained variance deviates more and more from the analytical result over time. This was also observed in earlier reports involving the product formula approach. Lastly, if we change Ω from 1 to 2, as in Fig. 1d the frequency of the oscillation of both mean and variance doubles, as expected from the analytical result. Additionally, we can also see that the sine-contribution to the variance in Fig. 1d is quadratically suppressed leading to a smaller minimum in contrast to Fig. 1b.



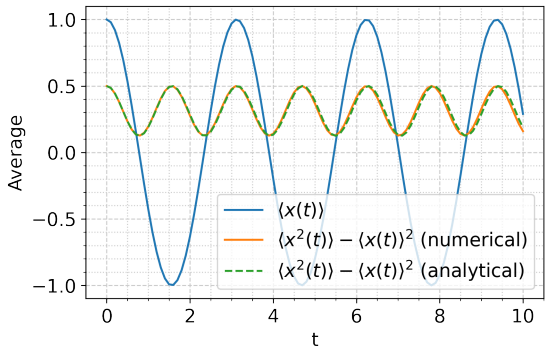
(a) Probability in space for $(\Omega, \sigma, x_0) = (1, 2, 0)$



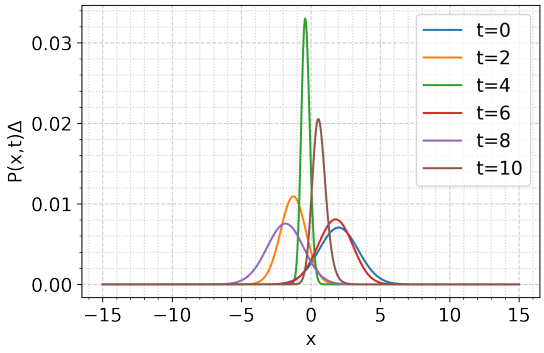
(b) Mean and variance in time for $(\Omega, \sigma, x_0) = (1, 2, 0)$



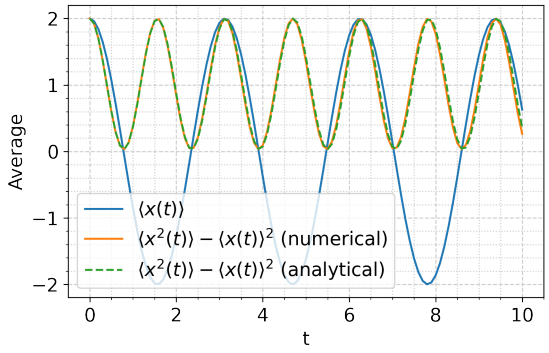
(c) Probability in space for $(\Omega, \sigma, x_0) = (2, 1, 1)$



(d) Mean and variance in time for $(\Omega, \sigma, x_0) = (2, 1, 1)$



(e) Probability in space for $(\Omega, \sigma, x_0) = (2, 2, 2)$



(f) Mean and variance in time for $(\Omega, \sigma, x_0) = (2, 2, 2)$

Figure 2. Time evolution of squeezed states for different initial conditions Ω, σ, x_0.

Discussion

In summary, I derived and implemented a simulation algorithm to numerically solve the Schrödinger equation for one-dimensional harmonic potentials using a product formula approach. Furthermore, I analytically obtained expectation value and variance of the time-dependent position operator which I subsequently compared to the numerical results. Overall, the analytical and numerical solutions match very well. I simulated the time evolution for initially coherent and squeezed states for which I made, in summary, following observations:

1. Coherent states evolve most classically. Their variance stays constant throughout the evolution and for the case of displacement the expectation value changes like the classical oscillator between the initial displacement x_0 and $-x_0$.
2. For squeezed states, the expectation value also evolves classically, however the variance oscillates in time. The period of oscillation is controlled by the frequency of the harmonic oscillator Hamiltonian Ω. The magnitude of the oscillation depends on the spread of the initial wave packet in position space, σ.
3. Both squeezed and coherent states fulfill the Heisenberg minimum uncertainty product $\Delta x \Delta p = 1/2$ at all times.
4. For large Ω a variance of almost 0 can be reached at certain times and for fast oscillation. At these times the position of the oscillator can be measured with highly increased accuracy.
5. The global error of the simulation can be controlled by increasing the time resolution.

Appendix

```python
# library imports
import numpy as np
import matplotlib.pyplot as plt
import matplotlib
font = {'size': 14}
matplotlib.rc('font', **font)

# parameters
delta = 0.025 # space step
L = 1201 # no. of space steps
L_half = (L-1) // 2 # half no. of space steps (used for splitting psi into pairs)
xs = np.linspace(-15, 15, L) # space grid (in steps of delta)

tau = 0.00025 # time step
m = 40_001 # no. of time steps
ts = np.round(np.linspace(0,10,m),5) # time grid (in steps of tau)

X = np.array([[0,1],[1,0]]) # Pauli X matrix
I = np.eye(2) # identity
a = tau/(4*delta**2)
A = np.cos(a)*I + 1j*np.sin(a)*X # e^(iaX)

# simulation
for omega, sigma, x0 in [(1,1,0),(1,1,1),(1,2,0),(2,1,1),(2,2,2)]: # showcases

    V = (xs * omega)**2 / 2  # potential energy function

    # initial wave function
    psi = (np.pi * sigma**2)**(-0.25)*np.exp(-(xs-x0)**2/(2*sigma**2)).astype(complex)

    psis = [] # track states
    psis.append(psi) # save initial state

    Ts = np.round(np.arange(0,10.1,0.1),1) # selected time points

    for t in ts[1:]: # ignore t=0 (as we tracked it already)

        # e^(-iTK2/2)e^(-iTK1/2)|psi>
        psi[:-1] = np.hstack([A @ v for v in np.split(psi[:-1], L_half)]).ravel()
        psi[1:] = np.hstack([A @ v for v in np.split(psi[1:], L_half)]).ravel()

        # e^(-iTV)|psi>
        psi = np.exp(-1j*tau*(delta**(-2) + V)) * psi

        # e^(-iTK1/2)e^(-iTK2/2)|psi>
        psi[1:] = np.hstack([A @ v for v in np.split(psi[1:], L_half)]).ravel()
```

```
        psi[:-1] = np.hstack([A @ v for v in np.split(psi[:-1], L_half)]).ravel()

        # save |psi>
        if t in Ts:
            psis.append(psi)

    psis = np.array(psis)
    probs = psis.real**2 + psis.imag**2 # calculate probabilities

    probs_sel = probs[np.where(Ts % 2 == 0)] # select probabilities for 0,2,4,..,10

    # Plot probability as function of position
    plt.figure(figsize=(6,4))
    plt.plot(xsrobs_sel.T*delta);
    plt.legend(['t=%d'%t for t in range(0,11,2)]);
    plt.xlabel('x');
    plt.ylabel(r'P(x,t)$\Delta$');
    plt.minorticks_on()
    plt.grid(which='major', color='#CCCCCC', linestyle='--')
    plt.grid(which='minor', color='#CCCCCC', linestyle=':')
    plt.tight_layout()
    plt.savefig(f'report/src/prob_k{omega}s{sigma}x{x0}.png', dpi=300)

    # calculate moments and var
    x1 = probs * xs
    x2 = probs * xs**2
    x1exp = np.sum(x1, axis=1) * delta # 1st moment
    x2exp = np.sum(x2, axis=1) * delta # 2nd moment
    var = x2exp - x1exp**2 # variance

    # analytical variance
    ana_var = 0.5 * (np.cos(omega*Ts)**2 * sigma**2 + np.sin(omega*Ts)**2 / (sigma**2*omega**2))

    # plot averages as function of time
    plt.figure(figsize=(6,4))
    plt.plot(Ts,x1exp);
    plt.plot(Ts,var);
    plt.plot(Ts,ana_var, '--')
    plt.legend([r'$\langle x(t) \rangle$', r'$\langle x^2(t) \rangle - \langle x(t) \rangle^2$ (
    numerical)', r'$\langle x^2(t) \rangle - \langle x(t) \rangle^2$ (analytical)']);
    plt.xlabel('t');
    plt.ylabel(r'Average');
    plt.minorticks_on()
    plt.grid(which='major', color='#CCCCCC', linestyle='--')
    plt.grid(which='minor', color='#CCCCCC', linestyle=':')
    plt.tight_layout()
    plt.savefig(f'report/src/avg_k{omega}s{sigma}x{x0}.png', dpi=300)
```