Report: Week 5

Quantum Information and Computing (2021/22)

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Continuous time-dependent Schrödinger equation

We consider the **time-dependent one-dimensional quantum harmonic oscillator** defined by the Hamiltonian:

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m}}_{K,\ \text{kin. term.}} + \underbrace{\frac{1}{2} m\omega^2 (\hat{x} - x_0(t))^2}_{V(t),\ \text{pot. term.}} \tag{1}$$

where $\omega = \sqrt{k/m}$ is the **angular frequency**, T is the characteristic time of the potential and $x_0(t) = t/T$, where $t \in [0 : T]$.

Given the ground state $|\psi_0\rangle = |n = 0\rangle$, we aim to solve the problem of finding the evolved state $|\psi(t)\rangle$ under $\hat{H}$:

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = \hat{H} |\psi\rangle \quad \rightarrow \quad |\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi_0\rangle \tag{2}$$

Numerical solution

Given a **space** interval $[-a, a]$ and a **time** interval $[t_0, t_f]$, we discretize both into N_x, N_t smaller intervals of width Δx, Δt,

$$\begin{aligned} x_i &= -a + i\Delta x \qquad & i &= 0, \dots, N_x \\ t_j &= t_0 + j\Delta t \qquad & j &= 0, \dots, N_t \end{aligned} \quad . \tag{3}$$

The formal solution of the Schrödinger equation for the wave function after a time step Δt is given by

$$|\psi(t + \Delta t)\rangle = e^{-i\hat{H}\Delta t} |\psi(t)\rangle \, . \tag{4}$$

We can exploit the **Baker-Campell-Hausdorff** approximation:

$$\exp\left(-i\hat{H}\Delta t\right) = \exp\left(-i\hat{V}\frac{\Delta t}{2}\right) \exp\left(-i\hat{K}\Delta t\right) \exp\left(-i\hat{V}\frac{\Delta t}{2}\right) + \mathcal{O}(\Delta t^3)$$

and apply each operator in the basis where it is diagonal using the **Fourier transform** $\mathcal{F}$. This is the **split-operator method**:

$$\psi_0(x_{i+1}, t_{j+1}) \approx e^{-i\frac{\Delta t}{2} V(x_i, t_j)} \mathcal{F}^{-1} e^{-i\Delta t K(p_i)} \mathcal{F} e^{-i\frac{\Delta t}{2} V(x_i, t_j)} \psi_0(x_i, t_j) \quad .$$

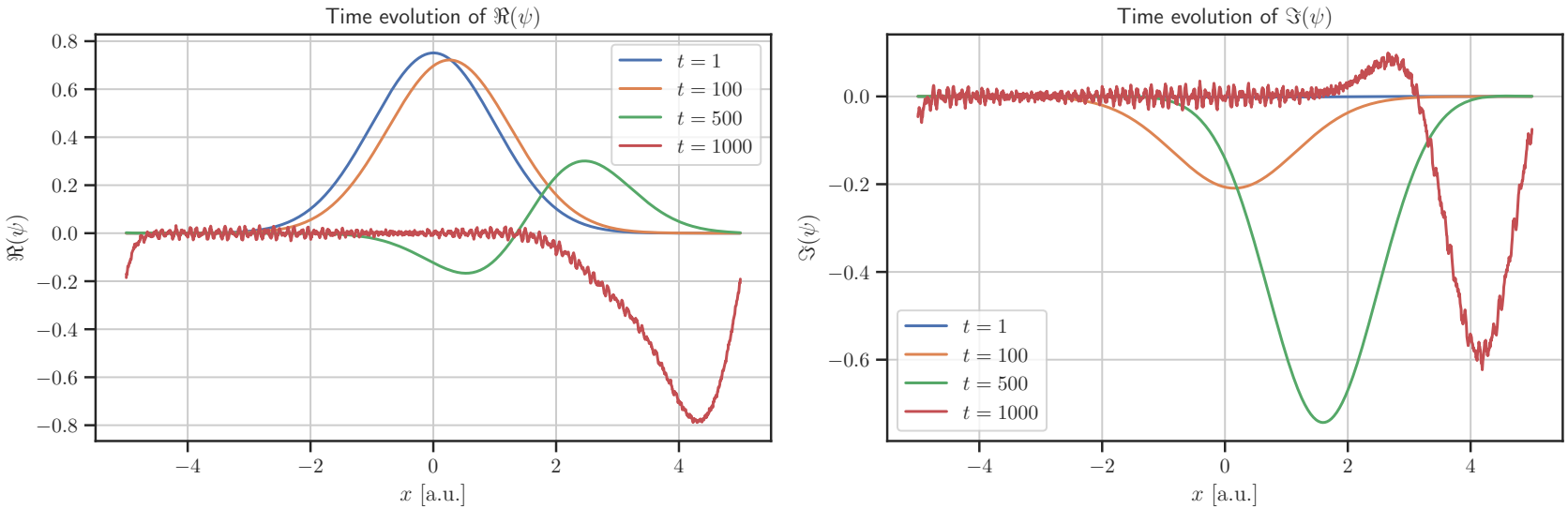
- Parameters are fed to the program as **user input**.
- We exploit the **dfftw_plan_dft_1d** and **dfftw_execute_dft** subroutines contained in the **FFTW3** library (normalization factor: $N_x^{-1/2}$).
- **Compile flags**: `-llapack -lfftw3 -lm -Wall`.

```
V = potential(N, x_max, m, omega, time, tau)
T = kinetic(N, x_max, m)

do ii=1,N+1
    psi(ii) = ZEXP(COMPLEX(0.0d0,-0.5d0*dt*V(ii))) * psi(ii)
end do

psi = FFT(psi)

do ii=1,N+1
    psi(ii) = ZEXP(COMPLEX(0.0d0,-1.0d0*dt*T(ii))) * psi(ii)
end do

psi = AFFT(psi)

do ii=1,N+1
    psi(ii) = ZEXP(COMPLEX(0.0d0,-0.5d0*dt*V(ii))) * psi(ii)
end do
```

Listing 1: Implementation of the time step evolution subroutine.

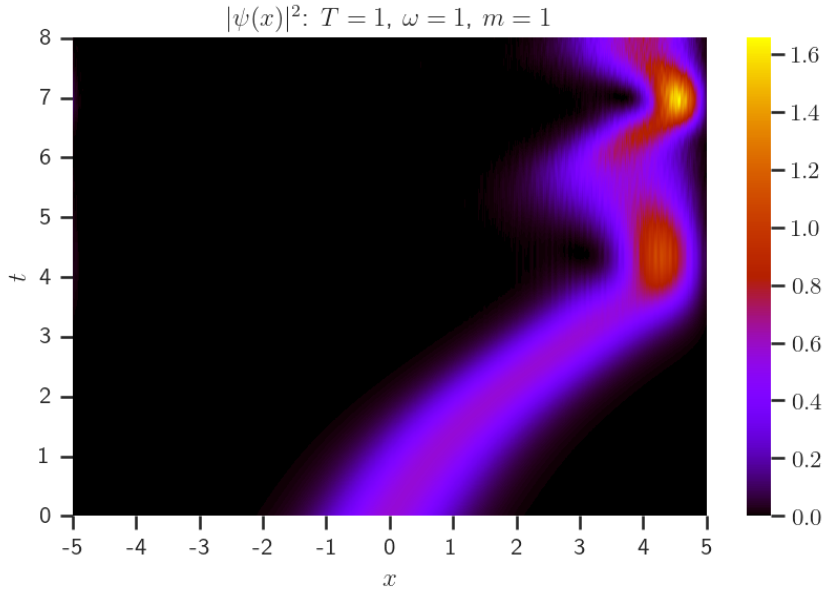
We plot the **real** and **imaginary** part of the wavefunction for different time steps.

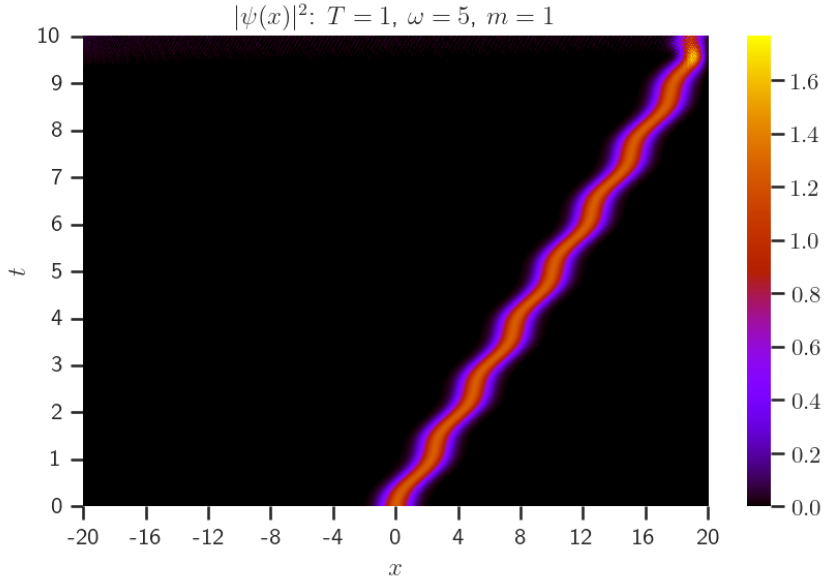
For higher time steps the wave function gets noisier since **boundary effects** arise: the wave start to propagate outside the simulation space range and **no more physical meaning** is associated to the simulation.

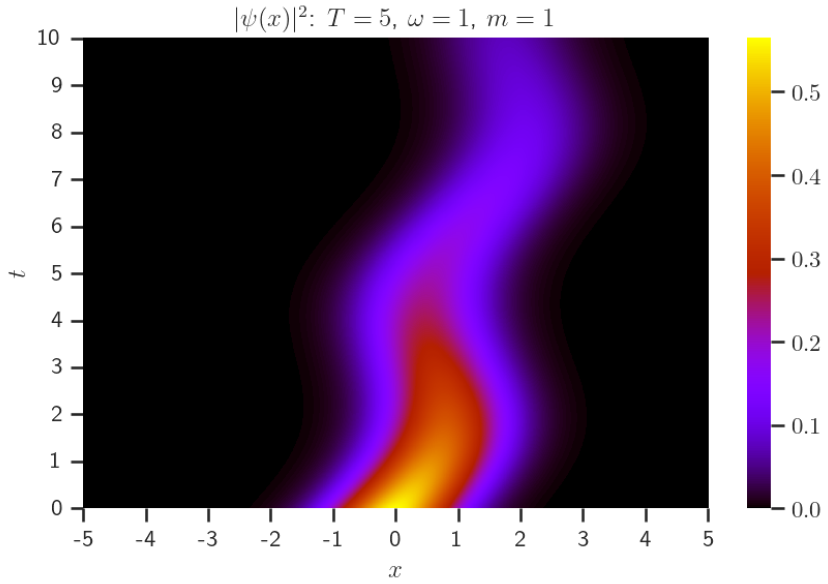


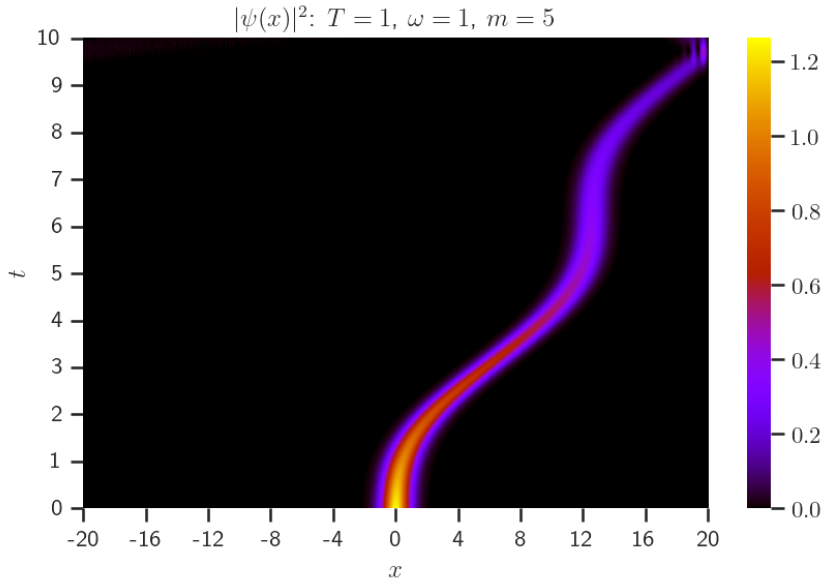
We plot the square modulus of the wavefunction $|\psi|^2$ in a heatmap: the most probable position moves **linearly** in time, as the potential **changes linearly**.

The oscillation is given by the harmonic part of the potential energy and can be increased by increasing ω.


$|\psi(x)|^2$: $T = 1$, $\omega = 1$, $m = 1$
t
x


$|\psi(x)|^2$: $T = 1$, $\omega = 5$, $m = 1$
t
x


$|\psi(x)|^2$: $T = 5$, $\omega = 1$, $m = 1$
t
x


$|\psi(x)|^2$: $T = 1$, $\omega = 1$, $m = 5$
t
x