Assignment 5

Quantum Information & Computing

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Theory

Formally, the Schrodinger equation solution can be evolved in time by a step Δt as

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

where $\hat{H}$ is a generic Hamiltonian s.t. $\hat{H} = \hat{V}(\hat{x}) + \hat{T}(\hat{p})$.

The **Suzuki-Trotter expansion** consists in writing the evolution operator as

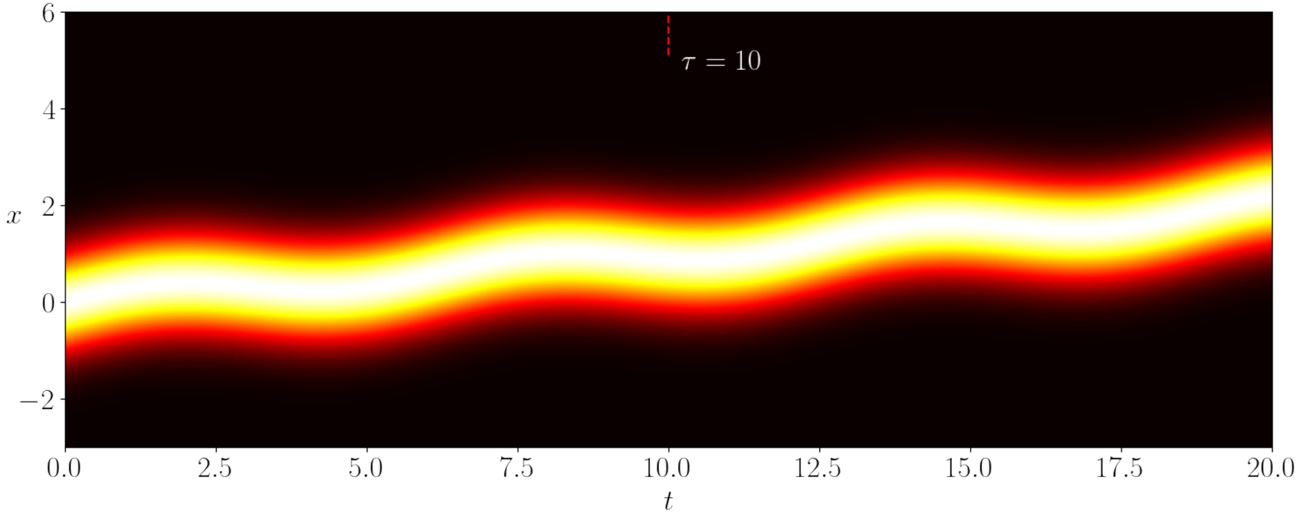
$$e^{-i\hat{H}\Delta t} = e^{-i\hat{V}\Delta t/2} e^{-i\hat{T}\Delta t} e^{-i\hat{V}\Delta t/2} + \mathcal{O}(\Delta t^3)$$

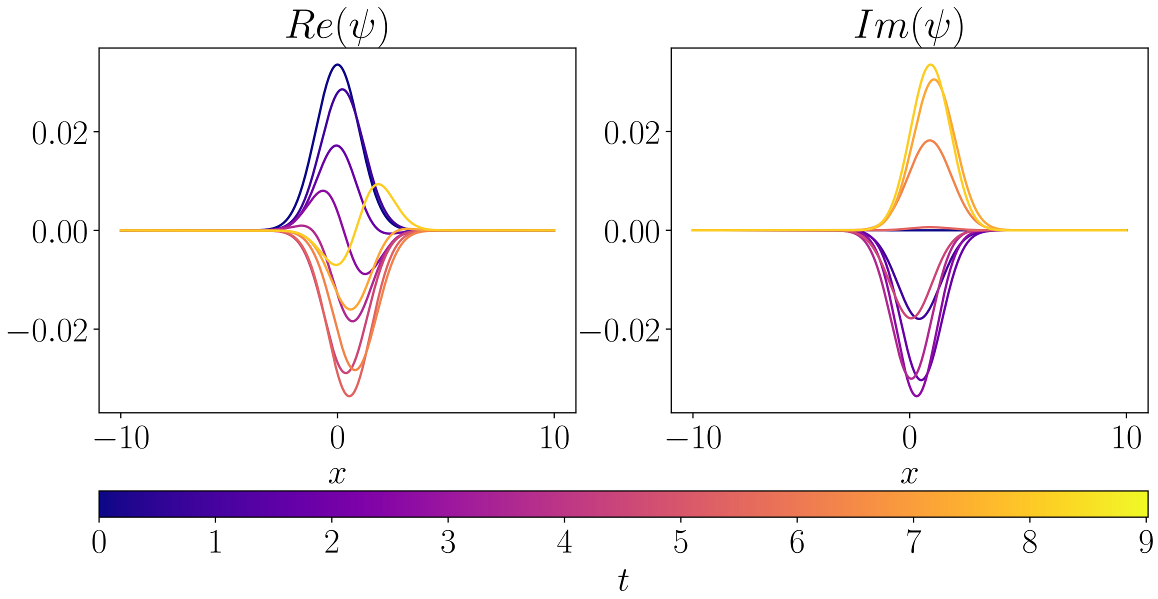
which is useful, since **each exponential term depends on a single variable**. The following algorithm takes advantage of such property.

It is convenient to apply each operator in the basis on which it appears diagonal. However, $\hat{V}$ and $\hat{T}$ depend on different coordinates, so one should perform at least a matrix-vector product. A generic change of basis would cost $\mathcal{O}(N^2)$. The solution to make this decomposition advantageous is to change coordinates $\hat{x} \longleftrightarrow \hat{p}$ with a Fourier Transform $\mathcal{F}$, which has cost $\mathcal{O}(N \log N)$ (using FFT).

$$\Rightarrow \quad e^{-i\hat{H}\Delta t}|\psi(x,t)\rangle \simeq e^{-i\hat{V}\Delta t/2} e^{-i\hat{T}\Delta t} e^{-i\hat{V}\Delta t/2}|\psi(x,t)\rangle = e^{-i\hat{V}\Delta t/2}\ \mathcal{F}^{-1}\ e^{-i\hat{T}\Delta t}\ \mathcal{F}\ e^{-i\hat{V}\Delta t/2}|\psi(x,t)\rangle$$

Results





$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\left(\hat{x} - \frac{t}{\tau}\right)^2$$

To test the simulation, we take as "default" parameters $x \in [-10, 10]$, $t \in [0, 20]$, with $\tau = 10$, $m = 1$.

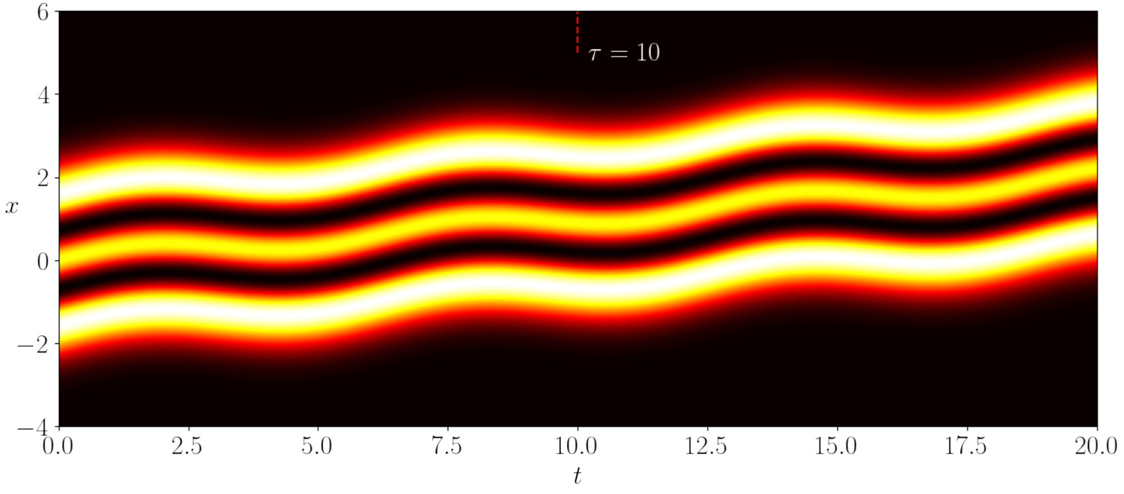
In the first picture you can see that **the probability density function drifts gradually towards higher values of** x, with an **oscillation component** that makes it 'wiggle' around the average linear drift.

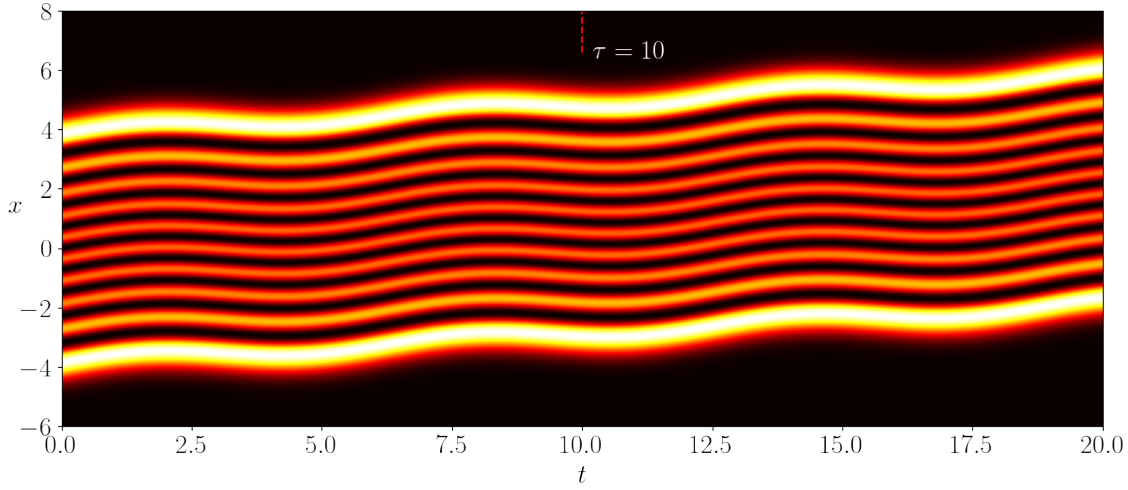
We expect the time sampling resolution to be a critical parameter, so we tried to test different values in a broad range.
Anyway, in this particular case it seems that sufficiently high values of time samples N_t produce similar results. Since we do not have any analytical solution to compare against the numerical simulation, we assess for $N_t = 10^4$.

Results

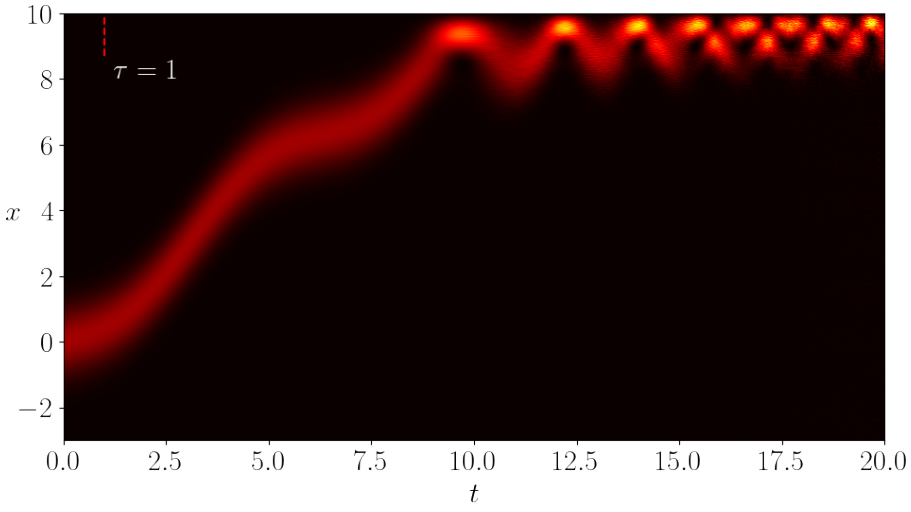
Not only the fundamental state

Of course, it is possible to compute the time evolution of other eigenstates. For instance, ψ_3 and ψ_{10} look this way:





Errors at boundaries

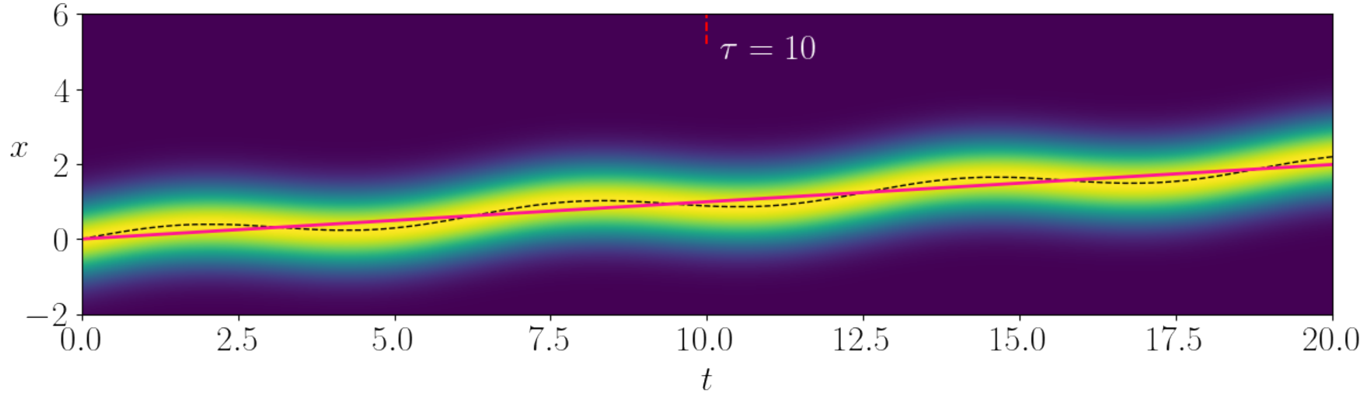


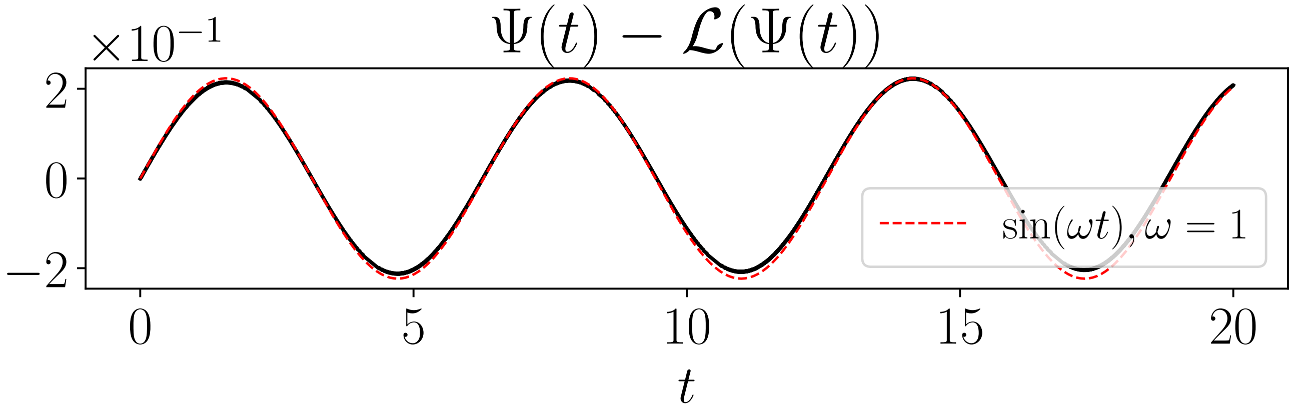
Lower values of the parameter τ will make the drift component more evident. For example, a value of $\tau = 1$ will make the wave function evolve quickly to the boundaries of the simulation domain, leading to bad results.

As long as we stay away from the boundaries, the behaviour of ψ is not anomalous.

Results // Characterizing the parameters

Consider again the foundamental eigenstate ψ_0. **Is it possible to characterize the drift and oscillation components of the evolving probability density function?**





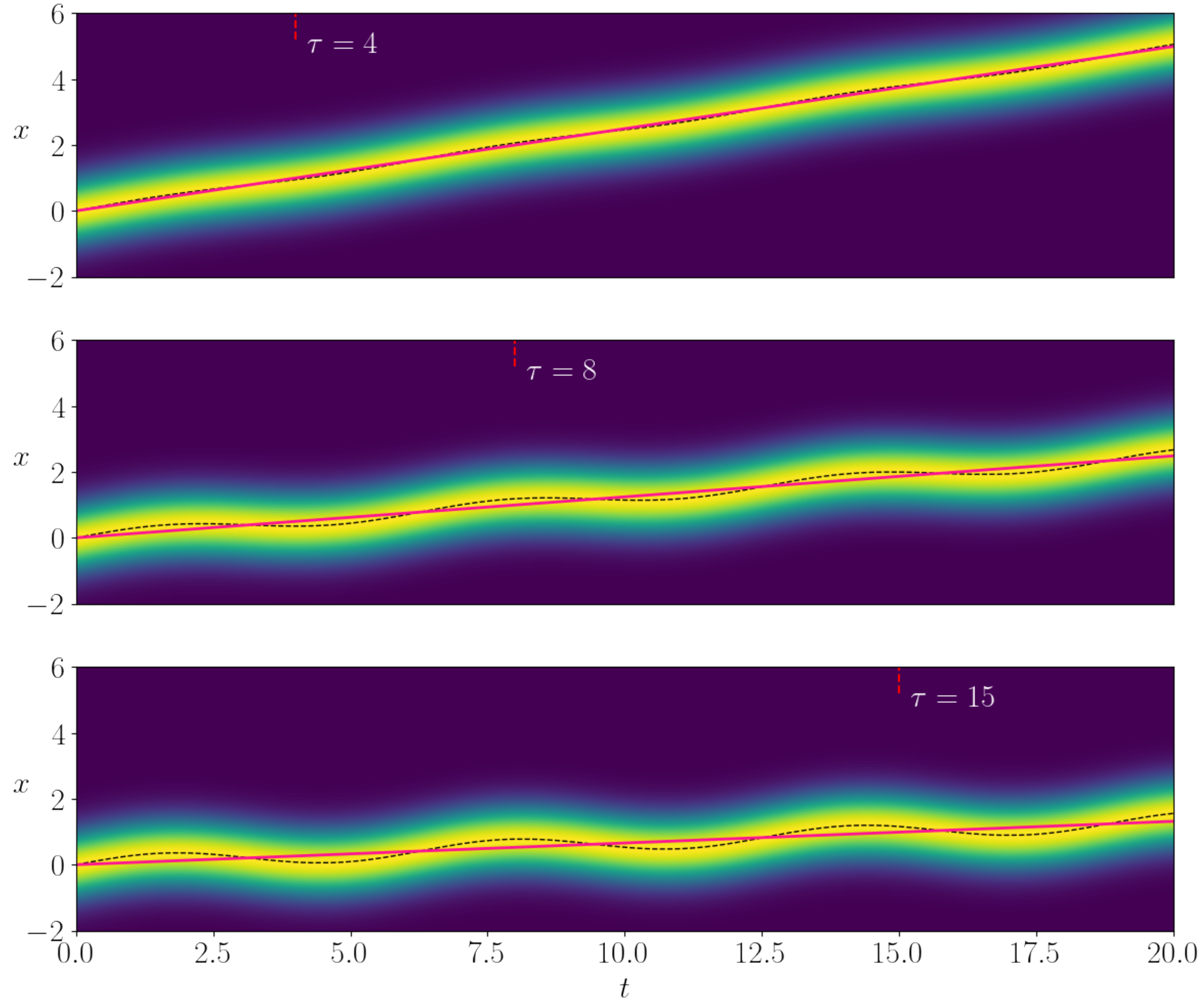
The black dashed line highlights the maximum of the probability density function $\Psi(t) = \max |\psi|^2$. By means of a linear fit, we can infer the linear drift component of the wavefunction, $\mathcal{L}(\Psi(t))$.

The angular coefficient of $\mathcal{L}(\Psi(t))$, in this example with $\tau = 10$, is

$$m = 0.0993313,$$

which is $\sim 1/\tau$.

Subtracting the drift component, we infer the oscillation component, which matches a $\sin$ oscillation with pulse ω_{osc} equal to the harmonic oscillator's ω.



The very same trand appears for simulations with different values of τ...

τ	m	$1/m$
4	0.2497	4.004
8	0.1244	8.038
10	0.0993	10.07
15	0.0659	15.17

... and ω. The following picture is an example for $\omega = 3$.