Assignment 5

Time-Dependent Schrödinger Equation

Quantum Information and Computing

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Theory

Numeric solution of the time-dependent Schrödinger equation

Time evolution: $\Psi(x, t) = e^{-i\hat{H}\Delta t}\Psi(x,0)$

Since the Hamiltonian does not commute with itself at different times, we can introduce a time-ordered product and rewrite the eigenstate as:
$\Psi(x, T) = \hat{U}(T, T/2)\hat{U}(T/2,0)\Psi(x,0)$

In order to implement a code to simulate the time dynamic of a time-dependent harmonic oscillator we had to use two approximations (for sufficiently small Δt):

1. The state evolution over a total time $T = n\Delta t$ can be written as:
   $\Psi_{n+1}(x) \sim e^{-i\hat{H}(n\Delta t)\Delta t}\Psi_n(x)$

2. Apply the Baker-Campbell-Hausdorff formula and split the contributions in the propagator

In this way, at the end we get: $\hat{U}(\Delta t)\Psi_n(x) = e^{-i\hat{V}(t)\frac{\Delta t}{2}}\mathcal{F}^{-1}e^{-i\hat{T}\Delta t}\mathcal{F}e^{-i\hat{V}(t)\frac{\Delta t}{2}}\Psi_n(x)$

Using Fourier transform, computational complexity: $O(NlogN)$

Workflow

Setting $m = \omega = \hbar = 1$ (oscillation period $T = 2\pi/\omega = 2\pi$) we consider the following time-dependent Hamiltonian to evolve our eigenstate:

$$\hat{H}(t) = \frac{\hat{p}^2}{2} + \frac{\omega^2(\hat{q} - q_0(t))^2}{2}, \ \ q_0(t) = \frac{t}{t_f}$$ controls the speed.

We performed the time evolution starting from the ground state in three regimes, fixing the simulation time $T = 20$ and changing t_f

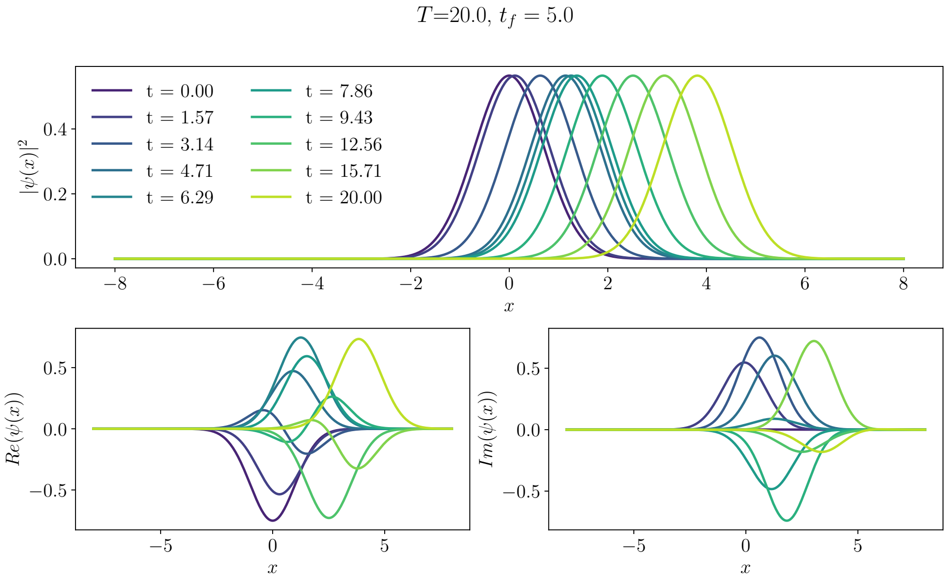
1. **Fast dynamics**, $t_f = 5$

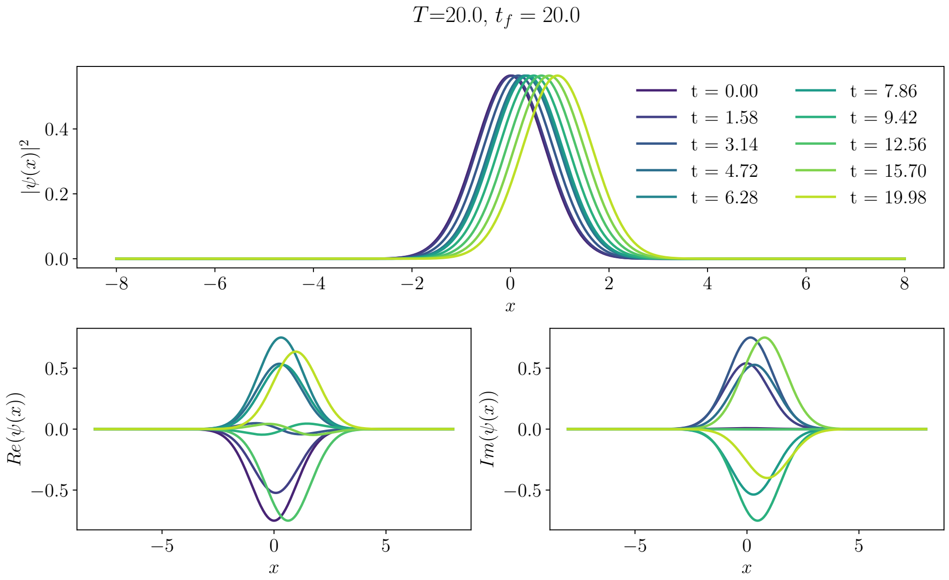
2. **Intermediate** (resonance) **dynamics**, $t_f = 20$

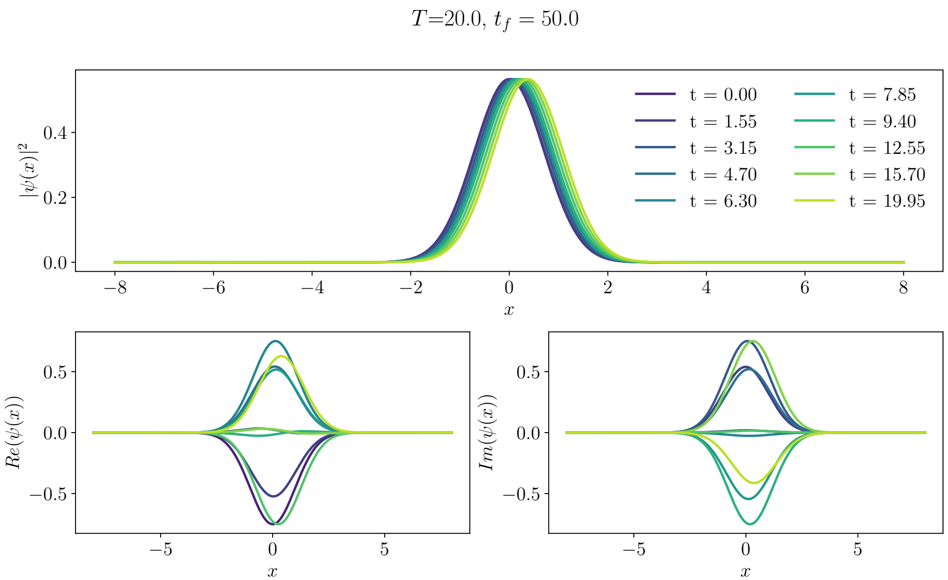
3. **Slow** (adiabatic) **dynamics**, $t_f = 50$

We will study the **motion of the wave packet in time** and the **evolution of the position expectation value.**

Comparison of different dynamics







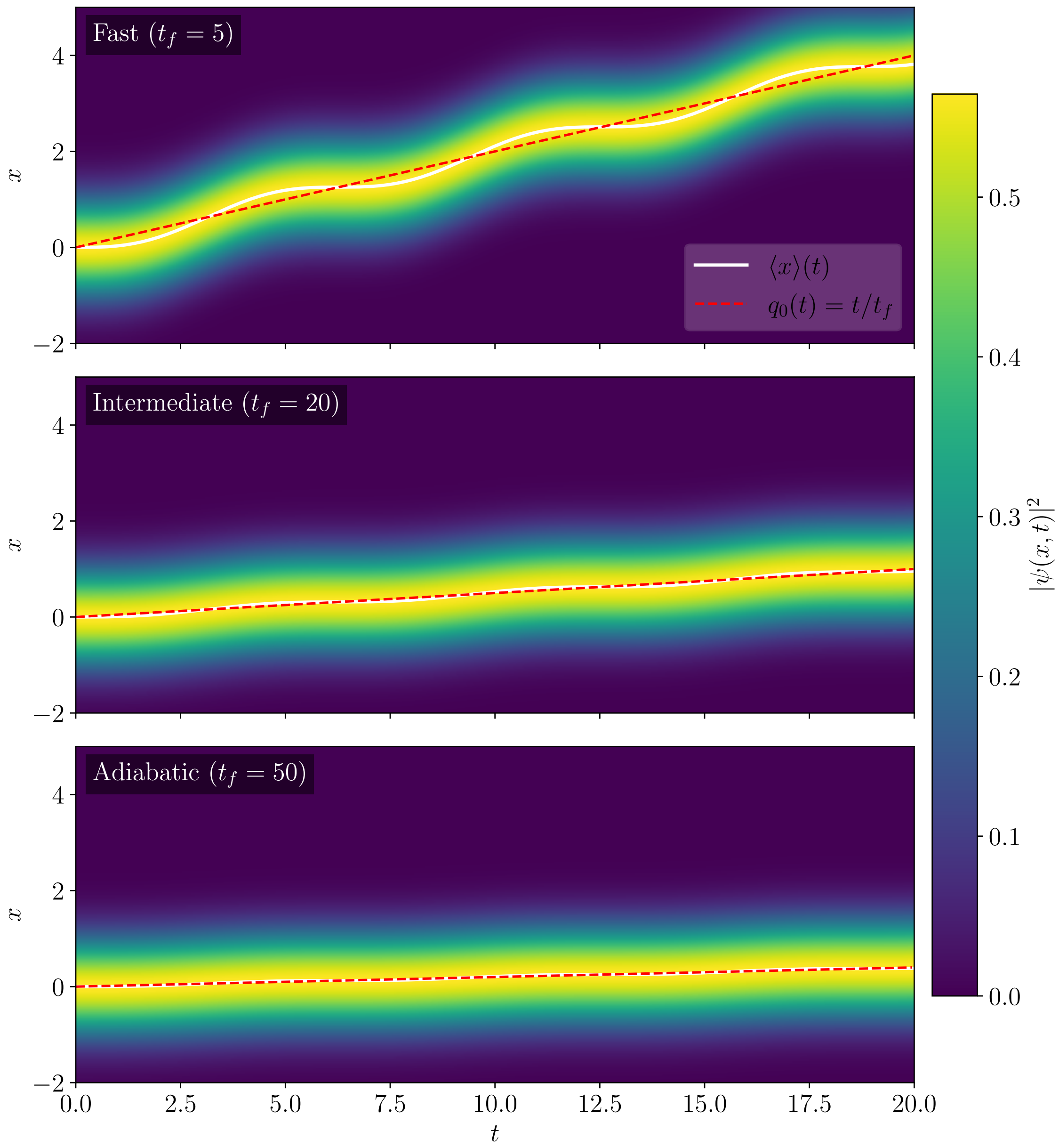
$|\psi|^2$ **(PDF):**

- Maintains Gaussian shape (Coherent State)
- Increasing t_f slows the potential, leading to adiabatic tracking

$Re(\psi), Im(\psi)$ **(Phase Dynamics):**

- **Momentum indicator:** Higher velocity, higher momentum, higher spatial frequency (denser oscillations, $\lambda = h/p$)
- **Phase:** Constant 90° phase shift between Real and Imaginary parts

Expectation value of the position



Fast ($t_f = 5$):

- Rapid potential shift overcomes system response time
- Large amplitude oscillations

Intermediate ($t_f = 20$):

- Coherent oscillations around the moving equilibrium

Adiabatic ($t_f = 50$):

- Perfect tracking of the ground state ($\langle x \rangle \approx q_0$) with negligible excitation

Physical and Coding parameters

There are several parameters that can control the dynamics:

Physical parameters:

- **Mass**: change the inertia of the particle into the potential
- **Frequency**: determine the oscillation period $T = 2\pi/\omega$
- **Speed** ($q_0(t) = t/t_f$): determine the regime one wants to investigate (critical parameter)

Coding parameters:

- **Grid points**: simply define the spacial and temporal resolution
- **Simulation time**: how long we let our system evolve
- **Steps** (dt, dx): affect numerical precision and stability (critical parameters)

Dynamics control

Eigenstates evolution:

- $V(x, t)$ is a rigid translation, the **instantaneous eigenstates** $\psi_n(x, t)$ do not change shape; they simply **translate rigidly** following the minimum $q_0(t) = t/t_f$