EXERCISE 5
CONTINUOUS TIME-DEPENDENT SCHRODINGER EQUATION

QUANTUM INFORMATION AND COMPUTING COURSE 2021/2022

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EXERCISE GOALS

Consider the one-dimensional Hamiltonian (translating harmonic oscillator

$$H = \frac{\hat{p}^2}{2} + \frac{1}{2}(\hat{x} - x_0(t))^2 \qquad x_0(t) = t/\mathrm{T},\ \ t \in [0{:}\mathrm{T}]$$

- Given $|\psi_0\rangle$ (the ground state of the Harmonic oscillator), compute $|\psi(t)\rangle$ for different values of T
- Plot the square norm of $|\psi(t)\rangle$ as a function of x at different times, and the average position of the particle as a function of t

IN THEORY…

- Potential shifts linearly in time, causing the wavefunction to translate
- Hamiltonian has kinetic component (depending solely on momenta) and potential component (depending solely on coordinante): the time evolution operator can be split symmetricly as follows:

$$\exp\left(-i\hat{H}\Delta t\right) = \exp\left(-i\hat{V}\Delta t/2\right)\exp\left(-i\hat{T}\Delta t\right)\exp\left(-i\hat{V}\Delta t/2\right)$$

- Therefore, by moving to coordinate/momenta domain the three operators on the left are diagonal: vector-vector multiplication instead of matrix-vector ($O(n)$ instead of $O(n^2)$). The domain change costs $O(n\ log\ n)$ for Fast Fourier Transform.

CODE DEVELOPEMENT

- Test FFT with Heaviside function
- Set discretization parameters:
  $x \in [-10,10],\ N_x = 2048,\ t \in [0,T],\ N_t = 2000$
- Definition of frequency domain

$$\omega \in \left[-{}^{\pi N_x}/_{20}, {}^{\pi N_x}/_{20}\right], N_\omega = 2048$$

  Rearranged according to documentation
- Exploit FFTW module with self-optimized parameters
- Normalize after each step

```
! Potential preparation
V = ((X-real(ii)*dt)**2)*(omega**2)/2.
V = complex(0.D0,-1.D0)*V*dt/2.
call ExpMatrix(V)

! Apply first potential term
psi_x = V*psi_x

! Move to momenta domain
call FT(plan, psi_x, psi_p)

! Apply kinetic term
psi_p = K*psi_p
psi_p = psi_p/cnorm(psi_p, dp)

! Move back to coord domain
call IFT(plan, psi_p, psi_x)

! Potential preparation
V = ((X-(real(ii)+0.5)*dt)**2)*(omega**2)/2.
V = complex(0.D0,-1.D0)*V*dt/2.
call ExpMatrix(V)

! Apply second potential term
psi_x = V*psi_x
psi_x = psi_x/cnorm(psi_x, dx)
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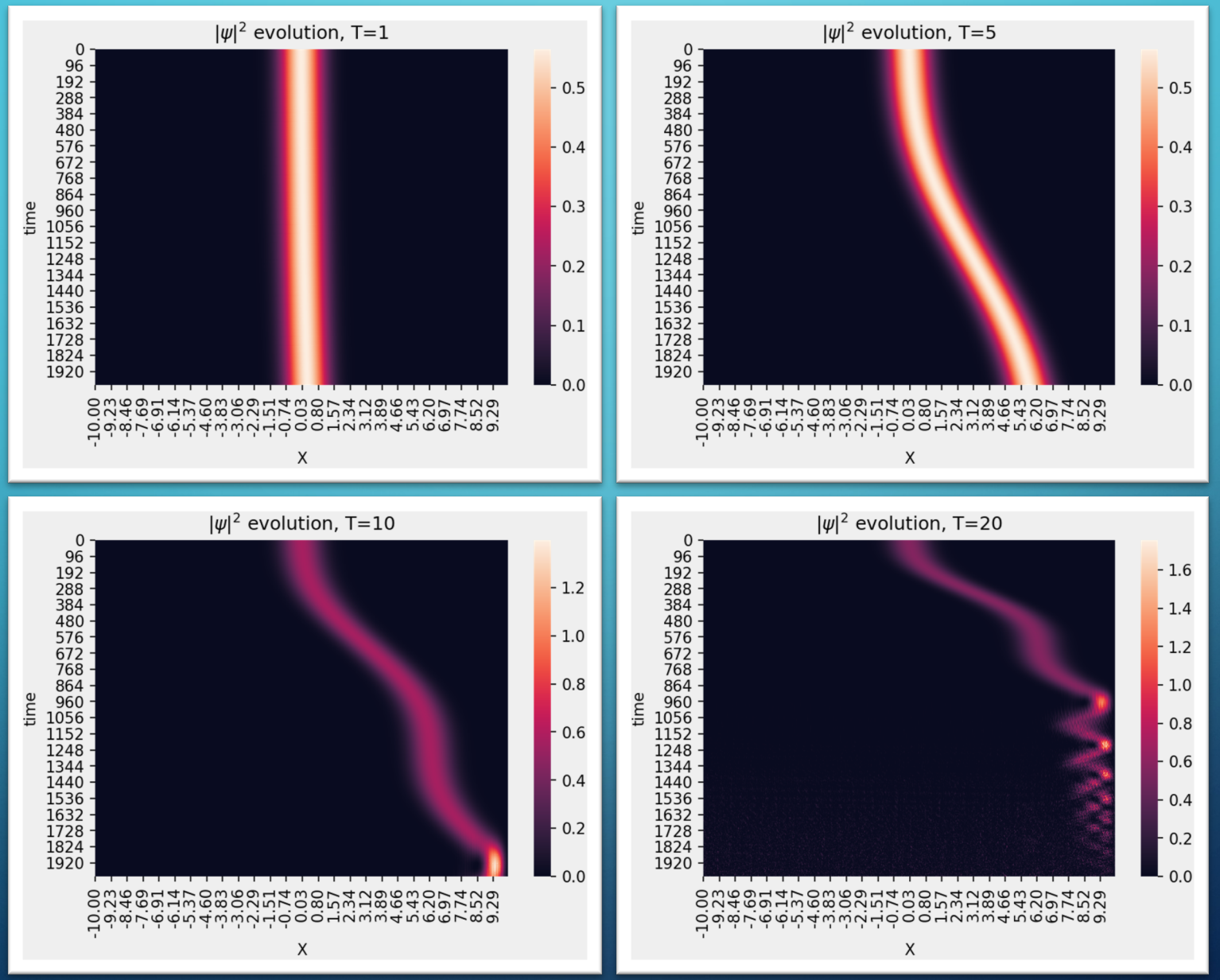
$|\psi|^2$ EVOLUTION IN TIME CHANGING T



ANIMATED $|\psi|^2$ EVOLUTION AND AVERAGE POSITION