Assignment 5

https://github.com/jchryssanthacopoulos/quantum_information/tree/main/assignment_5

Quantum Information and Computing
AA 2022–23

James Chryssanthacopoulos
6 December 2022

Università degli Studi di Padova

Time-Dependent Quantum System

Università degli Studi di Padova

- Goal is to solve 1D time-dependent quantum harmonic oscillator

$$\hat{H}\,|\Psi(x,t)\rangle = i\hbar\,|\Psi(x,t)\rangle\,, \quad \hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \frac{\omega^2}{2m}\left(\hat{x} - \frac{t}{T}\right)^2$$

- Problem was solved using **split operator method**, where state is evolved using

$$|\Psi(x, t+\Delta t)\rangle = e^{-\frac{i\hat{V}\Delta t}{2}}\mathcal{F}^{-1}e^{-i\hat{T}\Delta t}\mathcal{F}e^{-\frac{i\hat{V}\Delta t}{2}}\,|\Psi(x,t)\rangle$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ are the Fourier transform and its inverse, respectively ($\hbar = \omega = m = 1$ was used)

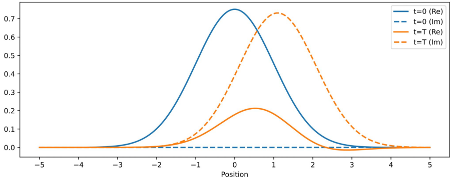
```
! multiply by potential part of Hamiltonian
do ii = 1, Nx
    V(ii) = potential(x_grid(ii), time, tmax)
    final_state(ii) = cexp(cmplx(0.0, -0.5 * V(ii) * dt)) * init_state(ii)
end do

! normalize
call normalize(final_state, dx)

! call FFT to go from coordinate space to momentum space
call dfftw_plan_dft_1d(plan, Nx, final_state, state_transform, -1, 64)
call dfftw_execute_dft(plan, final_state, state_transform)
call dfftw_destroy_plan(plan)
```

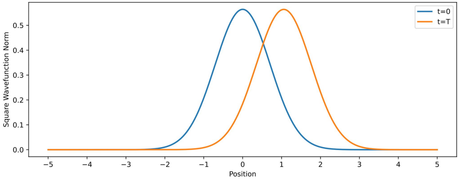
```
$ compiled/solve_time_dep_ho --xmin -15 --xmax 15 --tmax 10 --num_x_pts 100 --num_t_pts 100
 xmin = -15.000
 xmax = 15.000
 tmax = 10.000
 num_x_pts = 100
 num_t_pts = 100
 debug = F
 output_filename = solution.txt
```

- `fftw` library installed from source and used to compute FFT
- System simulated using discretization parameters and wavefunction saved to file, results analyzed in Jupyter notebook

Implementation and Solution

- $|\Psi(x,t)\rangle$ starts in ground state, $(\frac{1}{\pi})^{1/4}e^{-\frac{x^2}{2}}$
- Discretized momentum is given by $[0, \frac{2\pi}{L}, \ldots, \frac{\pi N}{L}, \frac{\pi(N-2)}{L}, \ldots, -\frac{2\pi}{L}]$, where N is number of x points and L is x range
- Wavefunction moves to right, developing complex phase, as expected





Wavefunction for Different T

Università degli Studi di Padova

- Expected position $\mathrm{E}[x](t)$ computed using $\sum_{i=1}^{N} x_i |\Psi(x_i, t)|^2 \Delta x$
- Result agrees well with theoretical result, $\mathrm{E}[x](t) = \frac{t}{T} - \sin\frac{t}{T}$
- Deviations from line decrease with increasing T