Assignment 5

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

Quantum Information and Computing
AA 2022–23

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Time-Dependent Quantum System

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

$$\hat{H}\,|\Psi(x,t)\rangle = i\hbar\frac{\partial}{\partial t}\,|\Psi(x,t)\rangle\,, \quad \hat{H} \equiv \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\left(\hat{x} - \frac{t}{T}\right)^2\,,\ t \in [0, T]$$

- 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)

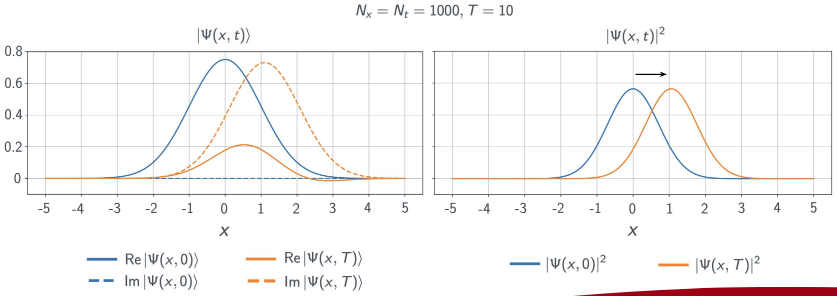
```
! multiply by potential part of Hamiltonian
do ii = 1, Nx
    V(ii) = potential(x_grid(ii), time, tmax)
    final_state(ii) = cexp(cmplx(0.0, -0.5 * V(ii) * dt)) * init_state(ii)
end do

! 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

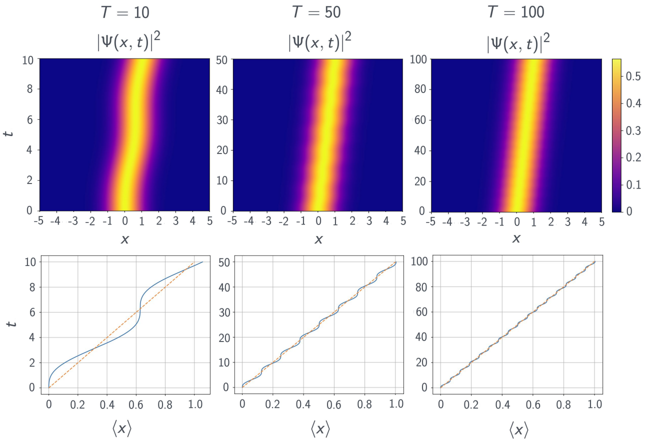
Implementation and Solution

- $|\Psi(x,t)\rangle$ starts in ground state, $\left(\frac{1}{\pi}\right)^{1/4} e^{-\frac{x^2}{2}}$
- Position and time discretized using N_x and N_t equispaced bins of size Δx and Δt
- Discretized momentum is $\left[0, \frac{2\pi}{L}, \ldots, \frac{\pi(N_x-2)}{L}, -\frac{\pi N_x}{L}, \ldots, -\frac{2\pi}{L}\right]$, where L is x range
- Wavefunction properly normalized by dividing by $\sqrt{\sum_{i=1}^{N_x} |\Psi(x_i,t)|^2 \Delta x}$
- Wavefunction moves to right, developing complex phase, as expected



Wavefunction for Different T

- Expected position $\langle x(t)\rangle$ computed using $\sum_{i=1}^{N_x} x_i |\Psi(x_i, t)|^2 \Delta x$
- Deviations from linear fit, $\langle x(t)\rangle - \frac{t}{T}$, decrease with increasing T



Position Oscillations

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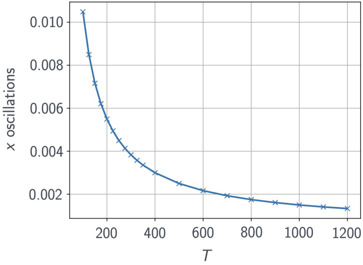
- Position oscillations decrease when T increases because when T is large, potential changes slowly (i.e., **adiabatic approximation**)
- Fit of oscillations to αT^{β} results in $\alpha = 0.60 \pm 0.03$ and $\beta = -0.88 \pm 0.01$



- Experiments showed that there are no oscillations with varying N_t

Self-Rating

- **Correctness.** Results seem sensible, but it is hard to know exactly without analytical wavefunction
- **Stability.** Code is numerically stable, but results sensitive to discretization
- **Accurate Discretization.** Error of split operator method is $\mathcal{O}(\Delta t^3)$. For $\Delta t \sim 1$, expected final state not reproduced
- **Flexibility.** Split operator method assumes $\hat{V}$ is only function of $\hat{x}$ and $\hat{T}$ is only function of $\hat{p}$, enabling exact diagonal representation
- **Efficiently.** Overall time complexity is $\mathcal{O}(N_t N_x \log N_x)$. It took ~ 8 s to solve using $N_x = N_t = 10^4$