Assignment 5

Time Dependent Schroedinger Equation

November 21st 2023

TIME DEPENDENT QUANTUM HARMONIC OSCILLATOR

Consider the time-dependent one-dimensional quantum harmonic oscillator defined by the Hamiltonian:

$$H = \frac{\hat{p}^2}{2m} + \frac{\omega^2(\hat{q} - q_0(t))^2}{2m}$$

with $q_0(t) = t/T$ and $t \in [0 : T]$. Given $|\Psi_0\rangle = |n = 0\rangle$ (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 q at different times, and the average position of the particle as a function of t.

TIME DEPENDENT SCHROEDINGER EQUATION

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t)$$

$$\hat{H} = \hat{T} + \hat{V}$$

Solution:

$$\Psi(x,t) = \hat{U}(t)\Psi(x,0) \quad \text{with} \quad \hat{U} = e^{-i\hat{H}t/\hbar}$$

WHAT if H(t) is time dependent?

The propagator can still be written in the same form, provided it describes the evolution in a time interval small enough.

$$\hat{U}(\Delta t) \sim e^{-i\hat{H}(t)\Delta t/\hbar}$$

The state evolution for a time $t = N\Delta t$ is obtained by successive application of the above operator, then:

$$\Psi(x,t) = \hat{U}(\Delta t)^N \Psi(x,0)$$

TIME DEPENDENT QUANTUM HARMONIC OSCILLATOR

$$
\begin{aligned}
H &= \frac{\hat{p}^2}{2m} + \frac{m\omega^2(\hat{x} - x_0(t))^2}{2} \\
&= \hat{T} + \hat{V}(t)
\end{aligned}
$$

(a) Write a program to compute the time evolution

(b) Plot the average position in time

TROTTER-SUZUKI DECOMPOSITION

$$
\begin{aligned}
\hat{U}(\Delta t) &= e^{-i\hat{H}(t)\Delta t/\hbar} \\
&= e^{-i\hat{T}\Delta t/\hbar} \quad e^{-i\hat{V}(t)\Delta t/\hbar} + \mathcal{O}(\Delta t^2) \qquad \text{Baker-Campbell-Hausdorff} \\
&= e^{-i\hat{V}(t)\Delta t/2\hbar} \quad e^{-i\hat{T}\Delta t/\hbar} \quad e^{-i\hat{V}(t)\Delta t/2\hbar} + \mathcal{O}(\Delta t^3) \qquad \text{TS}
\end{aligned}
$$

Since the representation of the kinetic operator is easier in the Fourier transformed space:

$$
\mathcal{F}\Psi(x) = \frac{1}{2\pi\hbar}\int e^{-ip_x x}\Psi(x)dx = \tilde{\Psi}(p_x)
$$

One can rewrite the expression for the propagator:

$$
\hat{U}(\Delta t) = e^{-i\hat{V}(t)\Delta t/2\hbar} \quad \mathcal{F}^{-1}e^{-i\hat{T}\Delta t/\hbar}\mathcal{F} \quad e^{-i\hat{V}(t)\Delta t/2\hbar}
$$

Code development:

A) Inputs: space interval ([min,max]), slice in space (Nslice), slice in time (Ntslice), duration of the simulation t_{sim}

B) Space discretization: $\Delta x = \dfrac{max - min}{Nslice}$ Time discretization: $\Delta t = \dfrac{t_{sim}}{Ntslice}$

C) Hamiltonian $H(t)$ discretization with finite difference method: eigenvalues and eigenvectors are stored

D) Evolved states (Nslice+1,Ntslice+1), first column initialized to ground state at time t=0

E) subroutine (def) for the split_step_method:

- Compute the potential operator in coordinate space for each time;
- Also kinetic part in the momentum space: it's discretized $p_n = \dfrac{2\pi n}{L}$, L is the space range

Check the normalization during each step

- Apply potential operator ;
- Fourier transform x—> px;
- Multiply by the kinetic operator;
- Fourier transform px —>x
- Multiply by potential;