QUANTUM INFORMATION AND COMPUTING

Assignment 5

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Time-dependent quantum harmonic oscillator

In this report, we use the split-step method to numerically predict how the ground state of a harmonic oscillator evolves with time when subjected to a time-dependent harmonic potential.

Theoretical background

Consider a one-dimensional quantum harmonic oscillator that evolves with time. The system is described by the Hamiltonian

$$\hat{H}(t) = \frac{\hat{p}^2}{2} + \frac{(\hat{x} - x(t))^2}{2}, \tag{1}$$

where $\hat{p}$, $\hat{x}$ are the operators for momentum and position respectively, and $x(t) = t/T$, where T is a constant. We assumed the mass of the particle, the reduced Planck constant and the angular frequency of the oscillator equal to 1, i.e. $\hbar = m = \omega = 1$.
Because the kinetic part of the Hamiltonian doesn't change over time, a useful method for numerically calculating the time evolution of a system governed by Equation (1) is the *split-step Fourier method*. With a time discretization $\{t_i\}_{i=1,..,N_t}$ with a sufficiently small time step dt, we operate under the assumption that the Hamiltonian remains constant throughout each time interval dt. Under this assumption, the time evolution of a state $\psi(x, t_i)$ during the time interval dt is given by

$$\psi(x, t_{i+1}) = e^{-i\hat{H}(t_i)dt}\psi(x, t_i). \tag{2}$$

The time evolution operators for each of the $N_t - 1$ time intervals, represented as $\hat{U}(t_i) = e^{-i\hat{H}(t_i)dt} = e^{-i(\hat{K}+\hat{V}(t_i))dt}$, incorporate both the kinetic operator $\hat{K}$ and the potential operator $\hat{V}(t_i)$ evaluated at the discretized time t_i. We can simplify this using the second-order *Trotter-Suzuki decomposition*, yielding:

$$e^{-i(\hat{K}+\hat{V}(t_i))dt} \simeq e^{-i\frac{\hat{V}(t_i)}{2}dt}e^{-i\hat{K}dt}e^{-i\frac{\hat{V}(t_i)}{2}dt} + O(dt^3). \tag{3}$$

As the kinetic operator depends solely on momentum, computing the second exponential term in Equation (3) becomes straightforward when applied within the momentum space. Specifically, this involves operating on the Fourier transform of the given wavefunction at time t_i, denoted as $\mathcal{F}\psi(x, t_i)$. By incorporating two Fourier transforms into the equation (3), the time evolution operator for each t_i, where $i = 1, .., N_t$, becomes the following

$$\hat{U}(t_i) \simeq e^{-i\frac{\hat{V}(t_i)}{2}dt}\mathcal{F}^{-1}e^{-i\hat{K}dt}\mathcal{F}e^{-i\frac{\hat{V}(t_i)}{2}dt} + O(dt^3). \tag{4}$$

Consider now a space discretization $\{x_j\}_{j=1,..,N_s}$ with a step size dx. Defining the length of the discretized space interval as $L = x_{N_s} - x_1$, the associated momentum discretization $\{p_i\}_{j=1,..,N_s}$ has a step size $dp = 2\pi/L$. We now proceed to discretize both the Hamiltonian and the wavefunction $\psi(x_j, t_i)$. The potential and kinetic operators are approximated by N_s-dimensional matrices. The potential matrix $V(t_i)$ is diagonal in the position space, while the kinetic matrix K is diagonal in the momentum space. By assembling all the discrete spatial values of $\psi(x_j, t_i)$ into an N_s-dimensional vector $\vec{\psi}(t_i)$, we arrive at the time evolution

rule utilized by the split-step method

$$\vec{\psi}(t_{i+1}) =\simeq e^{-i\frac{V(t_i)}{2}dt}\mathcal{F}_d^{-1}e^{-iKdt}\mathcal{F}_d e^{-i\frac{V(t_i)}{2}dt}\vec{\psi}(t_i) + O(dt^3), \tag{5}$$

where $\mathcal{F}_d$ represents the discrete Fourier transform.

Implementation

To enhance program flexibility, the code has been modularized into several functions saved in a separate file from the main one where parameters are defined, and results are displayed. Among these functions, we utilize one to calculate the eigenstates of the harmonic oscillator (initializing the split-step method with its ground state), another to compute the potential described in (1) (which can be substituted with different potentials depending on the objectives), a debugging function to ensure the normalization of a given quantum state, a function to calculate the energy (potential, kinetic, and total), and another to determine the expected value of position and its uncertainty for a given state. Lastly, there is a subroutine implementing the split-step method, taking the potential and its parameters as input, making its application straightforward for various potentials.

For all calculated integrals, Simpson's method is employed (with an error on the order of $O(dx^4)$, where dx is the spatial discretization step). To compute the discrete Fourier transform, we use the *fast Fourier transform* algorithm, with a runtime of $O(N \log N)$ when the number of spatial discretization points is a power of 2. Thus, we choose a spatial discretization in the interval [-10, 10] with $N_s = 2^{12}$ points. Regarding temporal discretization, a time step size of $dt = 0.05$ is used over a time window [0, 100].

The split-step method involves matrix-vector multiplications interspersed with Fourier transforms, as depicted in equation (5). This process is repeated for the number of temporal steps N_t. Matrix-vector multiplication typically has a runtime on the order of $O(N^2)$, where N is the size of the matrix and vector considered (in this case, $N = N_s$). However, it's important to note that in this specific scenario, the matrices involved are diagonal. As a result, the execution time of such a multiplication is equivalent to that of a vector-vector multiplication, i.e., on the order of $O(N)$. Then, the estimated runtime for the split-step method is on the order of $O(N_t \cdot N_s \log(N_s))$.

Results

In Figures 1, 2 and 3, the potential and the amplitude of wavefunction at times $t = 0$, $t = 50$, $t = 100$ are depicted, where the constant defining the potential is $T = 100$. In the attached gif provided with the assignment, it can be observed that as the potential starts to shift to the right, the amplitude of the wave function 'follows' the potential, oscillating within it.

Smaller values of T result in more pronounced oscillations, as demonstrated in Figures 4 and 5, illustrating the expected values of the particle's position over time along with its corresponding uncertainty.

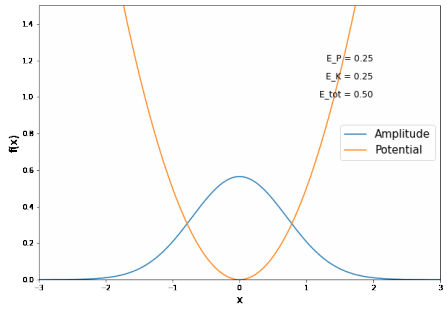

Figure 1: Potential ($T = 100$) and the amplitude of the wave function at the time $t = 0$.

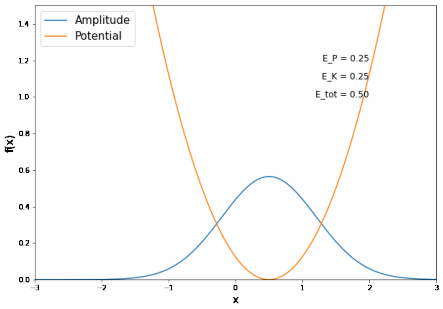

Figure 2: Potential ($T = 100$) and the amplitude of the wave function at the time $t = 50$.

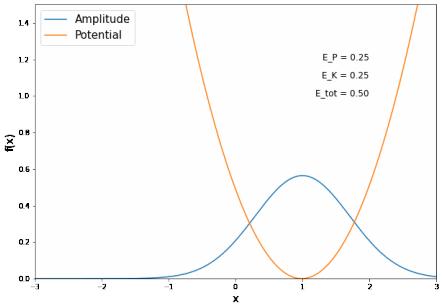

Figure 3: Potential ($T = 100$) and the amplitude of the wave function at the time $t = 100$.

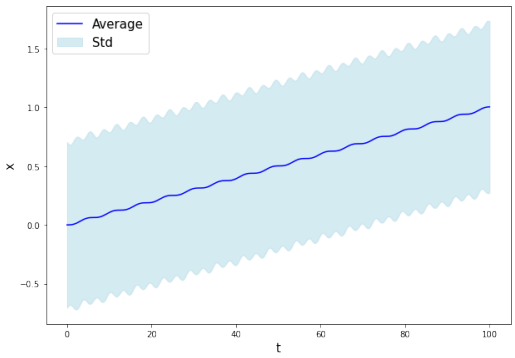

Figure 4: The expected value of the particle's position as a function of time, accompanied by its corresponding uncertainty. Here the potential is defined by $T = 100$.

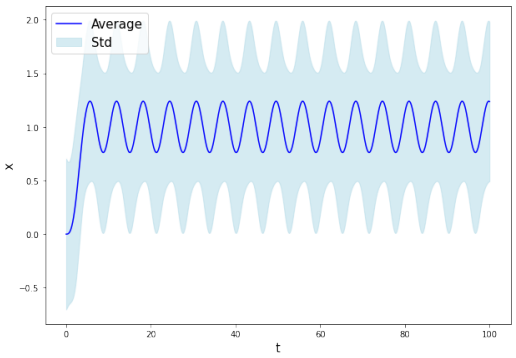

Figure 5: The expected value of the particle's position as a function of time, accompanied by its corresponding uncertainty. Here the potential is defined by $T = 5$.