PHYS 3120 Quantum Mechanics Term Project Proposal

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I. Research Question

The harmonic oscillator is a relevant problem in both classical and quantum mechanics. Our team aims to investigate the performance and accuracy of various time integration schemes for the quantum wave function in a harmonic oscillator. Furthermore, differences between the oscillations of a quantum and classical oscillator for both the damped and undamped cases will be studied.

II. Simulation description

Evaluating the behavior of a quantum wave function over time requires the solution of an initial value problem on the time-dependent Schrödinger equation, where the initial conditions will be a predefined superposition of the eigenstates of the undamped oscillator Hamiltonian. Starting with the undamped case, the known initial wave function will be propagated forward in time for a set amount of time and the full history of the probability distribution will be saved. After the simulation is completed, the result will be compared to the evolved time-independent solution that can be recovered from the initial superposition of eigenstates. This error analysis will serve to validate our numerical models against a known solution before considering the damped case. Once this step is completed, the same initial wave function will be propagated on the time-varying damped harmonic oscillator potential for the same time period. This will conclude the simulation phase of the project. During post-processing, the expected position of the particle at each time step will be computed from the probability density and compared to the position of an equivalent classical spring mass.

III. Required input physics

For the one-dimensional harmonic oscillator, the Hamiltonian is:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{1}$$

In (1), $\hat{p}$ is the momentum operator, m is the mass of the particle, ω is the angular frequency, and $\hat{x}$ is the position operator. The eigenstates of this Hamiltonian form a discrete set, with quantized energy levels given by

$$E_n = (n + \frac{1}{2})\hbar\omega \tag{2}$$

where n is a non-negative integer. These eigenstates form the basis for constructing any wave function of the system.

With dampening, the Hamiltonian for the oscillatory system is:

$$\hat{H} = \frac{\hat{p}^2}{2m}e^{-\alpha t} + \frac{1}{2}m\omega^2\hat{x}^2e^{\alpha t} \tag{3}$$

In (2), α is the dampening factor.

Given the initial state, $|\psi(0)\rangle$, the time-evolved state is expressed as:

$$|\psi(t)\rangle = e^{\frac{-i\hat{H}t}{\hbar}}|\psi(0)\rangle \tag{4}$$

The eigenstates of a Hamiltonian are the energy eigenstates, in which they satisfy the following relation:

$$\hat{H}|E\rangle = E|E\rangle \tag{5}$$

Using the relationship in (4), $\hat{H}$ can be replaced by its energy eigenstate and is plugged into (3). If the initial state is $|E\rangle$, equation (3) can be expanded into the following equation:

$$|\psi(t)\rangle = e^{\frac{-i\hat{H}t}{\hbar}}|E\rangle = e^{\frac{-iEt}{\hbar}}|E\rangle \tag{6}$$

IV. Literature review

McDonald's (2015) [1]research on considering systems in which friction is prevalent, in this case a damped harmonic oscillator, as inclusive in Hamiltonian dynamics displays an application in a Hamiltonian description for time-dependent forces.

[2] The harmonic oscillator is a fundamental concept in classical and quantum mechanics that describes systems subject to restoring forces proportional to displacement. The quantum harmonic oscillator Hamiltonian is shown in (1).

Lorentz initially proposed [3] the question of a time-dependent quantum oscillator at the 1911 Solvay Conference after Lecornu in 1895 began studies on a classical harmonic oscillator that had a time-dependent spring constant.

The one-dimensional harmonic oscillator can simulate how a particle experiences a potential energy that varies with position. Through this, we may determine the eigenstates and eigenvalues. A typical example of a system that behaves like harmonic oscillators includes the vibrations of nuclei within diatomic molecules.

[4] Because the harmonic oscillator has a known analytical solution, we may use this to determine and compare the error of varying numerical methods. This is how error analysis will be conducted against different time-integration schemes.

The total probability density can be determined through the inner product of the wave function with its complex conjugate. [4]

$$\langle \psi | \psi \rangle \tag{7}$$

The summation of all probability densities across the entire domain should equate to 1.

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1 \tag{8}$$

Where $\psi(x)$ is the wavefunction, and $|\psi(x)|^2$ represents the probability density of finding the particle at position x. Applicable numerical methods should conserve probability density, making this a necessary standard for quantifying error.

V. Computational methods

In order to evaluate the wave function at future times, the following time-integration schemes will be tested:

- Crank-Nicholson, from chapter 9 [5].
- 4th Order Runge-Kutta, from chapter 8 [5].
- Euler Integration, from chapter 8 [5].

Spatial derivatives can be computed using central differencing. Simpson's rule will be implemented according whenever integration over the spatial domain is required. The methods of central differencing and Simpson's rule will be obtained from chapter 5 of the text [5]. It should be noted that due to the predefined spacing of grid points, Gaussian quadrature is not possible for this problem.

VI. Simulation setup

The spatial domain will be defined in a predetermined number of equally spaced grid points at which the complex value of the wave function is defined. The width of the domain will be 5 times the classical turning point of an equivalent spring mass. The PDE solver will be run for 10 periods of the oscillator at constant time steps. The full state of the system will be stored as a $2N \times 1$ vector, where N is the number of grid points:

$$\mathbf{X} = \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_N \\ \frac{d\psi_1}{dt} \\ \vdots \\ \frac{d\psi_N}{dt} \end{bmatrix}.$$

The full time history of the solution can then be saved as a list of the aforementioned state vectors.

VII. Quantities to inspect

- $\psi(x)$: Wave function of the quantum particle, evaluated as a function of time and space. This gives the full state of the system at any point in time.
- $|\psi(x)|^2$: Probability density of the quantum particle, evaluated as a function of time and space, will be used to obtain the expected position of the particle.
- $\langle x \rangle$: Expected position of the quantum particle, evaluated as a function of time. This quantity will be relevant when comparing the quantum state to the position of an equivalent classical particle.
- $\langle E \rangle$: Expected energy of the particle, evaluated as a function of time. Energy can be tracked to observe the effect of damping on the system.

References

[1] McDONALD, K. T., "A damped Oscillator as a Hamiltonian System," *Joseph Henry Laboratory, Princeton University*, 2015.

[2] TOWNSEND, J. S., *A Modern Approach to Quantum Mechanics*, 2nd edition, University Science Books, 2013.

[3] LORENTZ, H., "La Theorie du Rayonnment et les Quanta," *"Discussion at the 1911 Solvay Conference"*, 1912, p. 450.

[4] VIKLUND, M. J., LINA, "Numerical approaches to solving the time-dependent Schrödinger equation with different potentials," *Uppsala Universitet*, 2016.

[5] NEWMAN, M., *Computational Physics*, 1st edition, CreateSpace Independent Publishing Platform, 2013.