NOTES ON PRINCIPLES OF QUANTUM MECHANICS THROUGH NUMERICS

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Introduction

The main idea of this short presentation is to illustrate some **fundamental principles of Quantum Mechanics** using numerics or numerical simulations: the **Heisenberg's Uncertainty Principle** and the **Quantum Tunneling**. The latter is achieved by propagating a wave packet on a given potential, i.e. *harmonic oscillator* and a *double well*, according to the time-dependent Schrödinger Equation:

$$\begin{aligned}
\mathrm{i}\frac{\partial \Psi(x,t)}{\partial t} &= \hat{H}(x,p)\Psi(x,t) \\
&= \left[\hat{T}(p) + \hat{V}(x)\right]\Psi(x,t)
\end{aligned}$$

The propagation is carried out by successive applications of the *time-evolution* operator at a given *time step* and using the Trotter approximation:

$$\begin{aligned}
\Psi(x,t) &= \mathrm{e}^{-\mathrm{i}t\hat{H}(x,p)}\Psi(x,0) \\
&= \mathrm{e}^{-\mathrm{i}t\left[\hat{T}(p)+\hat{V}(x)\right]}\Psi(x,0) \\
&\approx \mathrm{e}^{-\mathrm{i}t\hat{T}(p)}\mathrm{e}^{-\mathrm{i}t\hat{V}(x)}\Psi(x,0)
\end{aligned}$$

The initial wave function takes the form of a Gaussian wave packet:

$$\Psi(x,0) = N\mathrm{e}^{-\alpha(x-x_o)^2}$$

centered at a position $x = x_o$, and it is discretized on a grid of length L and a *grid step-size* Δx. The operators $\mathrm{e}^{-\mathrm{i}t\hat{T}(p)}$ and $\mathrm{e}^{-\mathrm{i}t\hat{V}(x)}$ are as well discretized on a grid in **momentum** and **real space**, respectively.
The operator associated to the potential is applied on the real space representation of the wave function, i.e. $\Psi(x,t)$, whereas the operator associated to the kinetic energy is applied on the momentum space representation, i.e. $\Psi(p,t)$. The latter is obtain via a **Fast Fourier Transformation**:

$$\Psi(p,t) = \mathscr{F}\left[\Psi(x,t)\right]$$

Therefore the wave function at a given time t can be written as:

$$\Psi(x,t) = \mathscr{F}^{-1}\left[\mathrm{e}^{-\mathrm{i}t\hat{T}(p)}\mathscr{F}\left[\,\mathrm{e}^{-\mathrm{i}t\hat{V}(x)}\Psi(x,0)\right]\right]$$

Uncertainty Principle

This section deals with the propagation of the wave packet in a *harmonic potential*:

$$V(x) = \frac{1}{2}m\omega^2 x^2$$

Both representations (real and momentum space) are shown. The objective is to comment on the following aspect related to the **Uncertainty Principle**:

- The particle is represented by a wave packet that has a certain distribution in real and momentum space.
- The momentum (velocity) is zero when the wave packet is at equilibrium position, and assumes a maximum value at the extremes.
- The momentum is positive when the wave packet propagates to the right.
- The momentum is negative when the wave packet propagates to the left.
- The wave packet in real space becomes wider at equilibrium, indicating a larger uncertainty in its position, while the momentum distribution becomes sharper, reaching its maximum velocity.
- The wave packet in real space becomes sharper at the edges, which indicates less uncertainty in its position, while the momentum distribution becomes wider around zero velocity.

Quantum Tunneling

In this section the wave packet is propagated in a *double-well potential* of the form:

$$V(x) = V_o\,\left[16x^4 - 8x^2 + 1\right]$$

where V_o corresponds to the height of the barrier separating both wells. This simulation illustrates the fact that the particle, represented by the Gaussian wave packet, is able to go through the barrier even though its energy E_o is smaller that that of the barrier:

$$E_o < V_o$$

To comment:

- In a classical world, if the energy E_o is smaller than the barrier V_o, the particle gets trapped in one of the wells without possibility of escaping.
- According to the laws of **Quantum Mechanics**, there is a non-zero probability to find the particle in a classically forbidden region, and this phenomenon is referred to as **Quantum Tunneling**.