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OscillR: a package for visualizing the quantum harmonic oscillator in R

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Abstract

The classical harmonic oscillator is a concept studied at the beginning of the advanced content on classical physics. That makes the study of the Quantum Harmonic Oscillator (QHO) a natural path. We present the `OscillR` package. The Quantum Harmonic Oscillator has been programmed in its statistical and dynamic versions for a truncated number of states. The graphs allow visualization of the probability of energies and positions, contributing to the community of Physicists users of R.

Keywords: Physics, quantum mechanics, data visualization, dynamics, R

Introduction

The development of the R programming language emerged around 1990, when two statisticians Ross Ihaka and Robert Gentleman decided to create a language based on the S language, where it was later expanded for further applications and developments. The advantages of R are: statistical computing and data analysis, open-source, large variety of libraries, cross-platform support, supports various data types, data cleansing, data wrangling, and web scraping, powerful graphic. Custom calculations that would be complex or time-consuming in other languages are easily manipulated in R [1].

The quantum oscillator is the classical harmonic quantum analogue in classical classical. In the quantum harmonic oscillator the energy becomes a Hamiltonian operator $\hat{H}$, whose observable corresponds to the total energy of the system, so that the moment becomes the moment operator and the operator position [2]. As quantum oscillations normally occur at a fixed set of individual energies, these energies are "quantized" and take on discrete values of semi-integer fractions, characteristic results of quantum systems:

$$\psi_n(x,t) = \left(X_0\, 2^n\, n!\, \sqrt{\pi}\right)^{-1/2} exp\left(\frac{-x^2}{X_0}\right) H_n\left(\frac{x}{X_0}\right) \exp\left(\frac{-iE_n t}{\hbar}\right).$$

In addition to the energies being quantized, these discrete energy levels are evenly spaced, and the lowest achievable energy (the ground state, n = 0), is not equal to the m intimate of potential well, which is called zero-point energy. For these reasons, the position and moment of the ground state oscillator are not fixed, but have a range of variation due to the Heisenberg's Uncertainty Principle [3]. The `OscillR` package was designed to enable the visualization of OHQ in two main cases the static form (no time evolution) and the dynamic form (time evolution).

This paper consists of the development of a new package, `OscillR`, for visualization of quantum harmonic oscillator solutions using R.

Methodology

The `OscillR` package was bilt in `R` language in order to enable the visualization of the Quantum Harmonic Oscillator in two main cases the static form (no time evolution) and dynamic form (time evolution). Tow main functions were built: `staticQHO(N, n, m_amu, f_inv_cm)` and `dynamicQHO(N, n, nt, psi_0_case)`.

Results

Oscillator mass and frequency are set by default (of course can be changed) but the user must set the number of basis states and the state index. The following example produces the output shown in Figure 1. The `staticHQO` function produces a couple of plots, one to show the eigenstate (with probability 100%); and the other describing the probability of particle location. The so called `dynamicQHO` function brings the visualization of the time evolution for the Quantum Harmonic Oscillator, the QHO dynamics. Its arguments are the number of basis states in a truncated representation (`N`); the index for a desired eigenstate (`N`); number of time points to be used (`nt`); the oscillator mass `m_amu` (in atomic mass units); the oscillator frequency (in cm^{-1}); the calculation time span in units of time 0 (`TimeSpan`); and the initial state preparation (`psi_0_case`). All the arguments are set to a default but the first ones (`N, n, nt`).

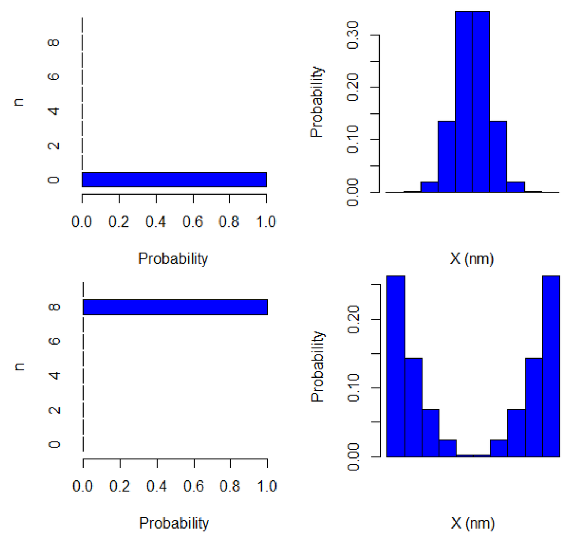

Figure 1: Eigenstate and probability vs location plots, N=10 basis states, highlighting the ground state and 8th exited state, respectively.

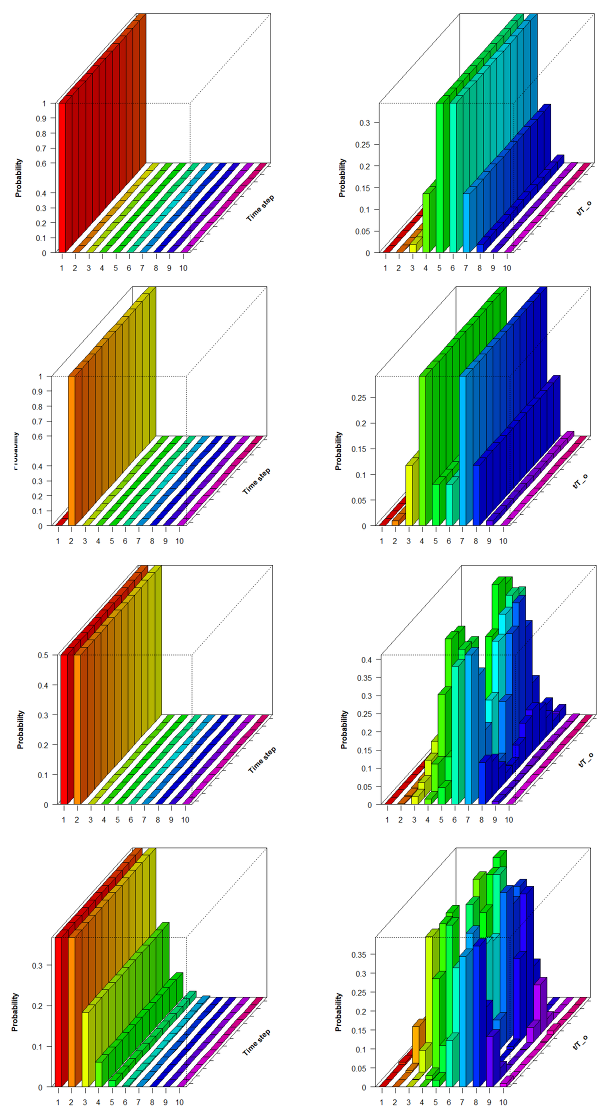

Figure 2: Probability of each eigenstate along time and the probability of each location along time, for the ground state, the firs excited state, a liner combination of stationary states and the Glauber state, respectively.

The output of `dynamicQHO` is a couple of 3D figures, as shown in Figure 2. That figure brings four initial states of preparation, the ground state, the first excited state, the linear combination of stationary states and the Glauber state. In each couple, the left graph shows the probability of each eigenstate along time; while the right one brings the probability of the location of the particle along time.

Conclusion

Visualizing data, patterns, forms and colours enhances the comprehension and the teaching and learning process. Specifically in quantum processes, data visualization is import due to the abstraction of the concepts and strangeness of the mechanics, compared to the macroscopic world.

The quantum harmonic oscillator is more easily understood with the help of data visualization, what is already done in so many languages. Now, the `OscillR` package, brings to R that application and contributes to the community of Physicists users of R.

References

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