# Ladder operators for the anharmonic oscillator

**Subject:** Non-commutative variables, pattern-matching.

## Introduction

Ladder operators, and more generally non-commuting operators of various types, appear in many contexts in Physics. In this problem we will learn how to implement basic non-commutative objects for fun and profit.

## Problem statement

We want to compute the first few energy levels of the anharmonic oscillator,[1] whose Hamiltonian in natural units is

$$\hat{H} = \frac{\hat{p}^2}{2} - \frac{\hat{x}^2}{2} + \frac{\hat{x}^4}{4}\,. \tag{1}$$

Working with a basis having a finite number $K$ of vectors $|\psi_i\rangle$ for $i = 1, 2, \ldots, K$, diagonalization of the $K \times K$ matrix $H_{ij} = \langle\psi_i|\,\hat{H}\,|\psi_j\rangle$ results in an approximate spectrum $E_i$ for $i = 1, \ldots, K$. If the basis was chosen appropriately, the lowest levels of this spectrum should be very close to the actual energy levels of the anharmonic oscillator.

Inspired by the harmonic case with Hamiltonian

$$\hat{H}_0 = \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2}\,, \tag{2}$$

[1] For example, this could be the initial guesses we use when solving the corresponding time-independent Schrödinger equation by the shooting method.

we will work with truncations of its Fock basis, $|n\rangle$ for $n = 0, 1, \ldots$. To construct this basis, introduce

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p}) \qquad , \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{p})\,, \tag{3}$$

and note that $[\hat{x}, \hat{p}] = i$ implies

$$[\hat{a}, \hat{a}^\dagger] = 1\,. \tag{4}$$

The Fock vacuum $|0\rangle$ is such that $\hat{a}\,|0\rangle = 0$, and the Fock basis is then defined by

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|0\rangle\ . \tag{5}$$

# Details

We want to implement variables $\hat{a}$ and $\hat{a}^\dagger$ whose product is not commutative, *i.e.* follows the commutation rule (4). `Mathematica` has a pre-implemented `NonCommutativeMultiply` function that provides some functionality, but it has some hidden `Attributes` that may complicate things. We will therefore define our own version using `CenterDot[x,y,...]`, which displays as $x{\cdot}y{\cdot}\ldots$.

First, define `CenterDot` to be linear and associative, so that for example

$$(\hat{a}^\dagger \cdot (\hat{a} + 3\hat{a}^\dagger)) \cdot \hat{a} \quad \mapsto \quad \hat{a}^\dagger \cdot \hat{a} \cdot \hat{a} + 3(\hat{a}^\dagger \cdot \hat{a}^\dagger \cdot \hat{a})\,, \tag{6}$$

where on the right hand side the factor of 3 is outside `CenterDot`. Next, define `CenterDot` to always respect normal order, so that following (4) we have

$$\cdots \hat{a} \cdot \hat{a}^\dagger \cdots \mapsto \cdots (1 + \hat{a}^\dagger \cdot \hat{a}) \cdots\,. \tag{7}$$

**Note:** Be careful about the identity opeator above! How is it represented in your implementation?

To check your implementation, define $\hat{x}$ and $\hat{p}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$ from (3), and make sure that the harmonic oscillator Hamiltonian (2) turns out to be

$$\hat{H}_0 = \hat{a}^\dagger \cdot \hat{a} + \tfrac{1}{2}\,. \tag{8}$$

**Note:** Remember to write $\hat{x}^2$ and $\hat{p}^2$ as $\hat{x} \cdot \hat{x}$ and $\hat{p} \cdot \hat{p}$, respectively.

You can now easily rewrite the anharmonic oscillator's Hamiltonian (1) in terms of $\hat{a}$ and $\hat{a}^\dagger$. What do you get?

Moving on, define the Fock basis through (5), so that for example

$$\texttt{State}[3] \mapsto \frac{\hat{a}^\dagger \cdot \hat{a}^\dagger \cdot \hat{a}^\dagger \cdot |0\rangle}{\sqrt{6}} \qquad , \qquad \texttt{Costate}[4] \mapsto \frac{\langle 0| \cdot \hat{a} \cdot \hat{a} \cdot \hat{a} \cdot \hat{a}}{\sqrt{24}} \,. \tag{9}$$

Adding the conditions $\hat{a}\cdot|0\rangle = 0 = \langle 0|\cdot\hat{a}^\dagger$, as well as the vacuum normalization $\langle 0|0\rangle = 1$, check explicitly that this basis is properly orthonormalized to $\langle n|m\rangle = \delta_{nm}$.

We can further check the Fock basis implementation by making sure it diagonalizes the harmonic oscillator Hamiltonian (8). For this, compute its matrix elements taking $K = 5$, to obtain

$$\left\langle n\middle|\hat{H}_0\middle|m\right\rangle = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{7}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{9}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{11}{2} \end{pmatrix} . \tag{10}$$

We are finally ready to compute an approximation to the anharmonic oscillator's lowest energy levels: explicitly obtain the $H_{nm}$ matrix elements from the anharmonic oscillator's Hamiltonian for some fixed small value of $K$, then use `Eigenvalues` to calculate the spectrum. Can you estimate the truncation error we are incurring in? How far can you take $K$? Can you explain why the process becomes slower and slower as $K$ increases? Estimate the number of operations required to compute $H_{nm}$ and see how it scales with $K$.

Now take a look at the $H_{nm}$ matrix you have just computed. What can you say about its structure? Can you guess its general form? Let `Mathematica` help you: obtain the first 6 elements in each non-vanishing diagonal, and then use `FindSequenceFunction` or `InterpolatingPolynomial` to generalize these numbers (you can try this out first with the values of the harmonic case, (10), to make sure you can reproduce $(H_0)_{nm} = \delta_{nm}(n + \frac{1}{2})$ as expected).

Once you have a generic form for $H_{nm}$, you can take much larger values of $K$ to compute the spectrum! Write a function that computes all the energy levels for a given $K$, and returns those for which the absolute or relative error is bounded by some small value (you can check self-consistency by playing with different values of $K$).

Now, can we do better and avoid all guesswork? Note that the Fock basis satisfies

$$\hat{a} \cdot |n\rangle = \sqrt{n}\,|n-1\rangle \qquad \text{and} \qquad \hat{a}^\dagger \cdot |n\rangle = \sqrt{n+1}\,|n+1\rangle \ . \tag{11}$$

Using these rules in conjunction with the orthonormalization condition $\langle n|m\rangle = \delta_{nm}$, instead of the explicit construction (5), recover the symbolic expression you guessed for $H_{nm}$ before.

# Useful functions

You may find it useful to read the `Mathematica` help pages of the following functions:

- **Displaying functions:** `NonCommutativeMultiply`, `CenterDot`, `Bra`, `Ket`, ...
- **Matrix functions:** `Eigenvalues`, `Diagonal`, ...
- **Other functions:** `ClearAll`, `SetAttributes`, `FindSequenceFunction`, `InterpolatingPolynomial`, ...