Project 2
Numerical Investigation of Quantum Systems

1 Introduction

In this project, we approximately numerically diagonalize the quantum anharmonic oscillator hamiltonian using what we already know about the quantum harmonic oscillator.

2 The quantum harmonic oscillator

The **quantum harmonic oscillator** is defined by the following Hamiltonian given in non-dimensionalized form:

$$\hat{H}_0 = \frac{1}{2}(\hat{p}^2 + \hat{x}^2) \tag{1}$$

where $\hat{x}$ and $\hat{p}$ satisfy the **canonical commutation relation**

$$[\hat{x}, \hat{p}] = i. \tag{2}$$

Here we work in units where $\hbar = 1$. It is possible to diagonalize the Hamiltonian by purely algebraic means by introducing the **raising operator** $\hat{a}_+$ and **lowering operator** $\hat{a}_-$, defined by

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

$$\hat{a}_- = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p}). \tag{4}$$

In particular, by some clever argumentation, one can show that there exists an orthonormal basis

$$B_0 = \{|0\rangle, |1\rangle, \dots\} \tag{5}$$

for the Hilbert space of this system satisfying

$$\hat{a}_+|n\rangle = \sqrt{n+1}|n+1\rangle \tag{6}$$

$$\hat{a}_-|n\rangle = \sqrt{n}|n-1\rangle \tag{7}$$

and moreover that the hamiltonian can be written in terms of the raising and lowering operators as

$$\hat{H}_0 = \hat{a}_+\hat{a}_- + \frac{1}{2}\hat{I}, \tag{8}$$

from which it follows that

$$\hat{H}_0|n\rangle = (n + \tfrac{1}{2})|n\rangle. \tag{9}$$

In other words, the Hamiltonian is diagonal in the basis B_0, and the eigenvalue E_n corresponding to eigenvector $|n\rangle$ is

$$E_n = n + \tfrac{1}{2} \tag{10}$$

In fact, the matrix elements of $\hat{H}_0$ in the basis B_0 are

$$\langle m|\hat{H}_0|n\rangle = (n + \tfrac{1}{2})\delta_{mn} \tag{11}$$

$$\langle m|\hat{a}_+|n\rangle = \sqrt{n+1}\delta_{m,n+1} \tag{12}$$

$$\langle m|\hat{a}_-|n\rangle = \sqrt{n}\delta_{m,n-1} \tag{13}$$

These expressions give the matrix representations of these three operators in the basis B_0, and if one restricts attention to the subspace spanned by the basis vectors $|0\rangle, |1\rangle, \dots, |N\rangle$, then one can write $(N+1)\times(N+1)$ matrix representations of these operators restricted to that subspace. These matrix representations can then be put on computer, e.g. as numpy arrays in Python, and one can use them to numerically compute eigenvectors and eigenvalues.

2.1 Wavefunctions

Note that it is also possible to think of the vectors $|n\rangle$ in the basis B_0 as **wavefunctions** instead of in the abstract, and in factor the wavefunction ψ_n that corresponds to $|n\rangle$ is

$$\psi_n(x) = (2^n n! \sqrt{pi})^{-1/2} e^{-x^2/2} h_n(x) \tag{14}$$

where h_n is the n^{th} Hermite polynomial which can be determine according to the following definitions of the first two:

$$h_0(x) = 1 \tag{15}$$

$$h_1(x) = 2x \tag{16}$$

$$\tag{17}$$

and the recursion relation

$$h_{n+1}(x) = 2xh_n(x) - 2nh_{n-1}(x). \tag{18}$$

3 The quantum anharmonic oscillator

Let $\lambda > 0$, and consider the **quantum anharmonic oscillator** defined by

$$\hat{H}_\lambda = \hat{H}_0 + \lambda \hat{x}^4. \tag{19}$$

Unfortunately, the elegant algebraic method used to diagonalize the quantum harmonic oscillator hamiltonian does not work for this modified hamiltonian. Instead, we can find approximate numerical eigenvectors and eigenvalues according to the following scheme.

1. Determine the matrix elements of $\hat{H}_\lambda$ in the harmonic oscillator basis B_0 using raising and lowering operators.
2. Restrict attention to the subspace spanned by the basis

   $$B_{0,N} = \{|0\rangle, |1\rangle, \ldots, |N\rangle\} \tag{20}$$

   and find the matrix representation of $\hat{H}$ in this bases – an $(N+1)\times(N+1)$ matrix.
3. Using Python to numerically diagonalize this matrix representation.
4. Find N large enough that the eigenvalues and eigenvectors begin to converge to stable values which are approximations to the true eigenvalues and eigenvectors.

4 Assignments

1. Show that the operators $\hat{x}^2$ and $\hat{x}^4$ have the following matrix elements in the harmonic oscillator basis:

   $$\langle n|\hat{x}^2|m\rangle = (n+1/2)\delta_{nm} + \tfrac{1}{2}\sqrt{(n+1)(n+2)}\,\delta_{n,m-2} + \tfrac{1}{2}\sqrt{(n-1)n}\,\delta_{n,m+2} \tag{21}$$

   $$\begin{aligned}\langle n|\hat{x}^4|m\rangle = {} & \tfrac{1}{4}\Big(6n^2+6n+3\Big)\delta_{nm} + \sqrt{(n+1)(n+2)}\,\Big(n+\tfrac{3}{2}\Big)\delta_{n,m-2} + \\ & + \sqrt{(n-1)n}\,\Big(n-\tfrac{1}{2}\Big)\delta_{n,m+2} + \tfrac{1}{4}\sqrt{(n+1)(n+2)(n+3)(n+4)}\,\delta_{n,m-4} + \\ & + \tfrac{1}{4}\sqrt{(n-3)(n-2)(n-1)n}\,\delta_{n,m+4}.\end{aligned} \tag{22}$$

2. Solve the anharmonic oscillator eigenvalue problem written in the harmonic oscillator basis for at least the first four energy levels. The design and implementation of efficient eigenvalue algorithms is a sophisticated topic. Therefore, we recommend you use an optimized eigenvalue solver from a well-known numerical library or computational environment.

   You are encouraged to look use the methods built into NumPy and SciPy for computing the eigenvalues and eigenvectors of real, symmetric matrices. As an additional hint for those using Python, we also mention that the function “hermval” from NumPy offers an easy solution to compute the eigenfunctions $\psi_n(x)$ from the eigenvectors of the matrix representation of the hamiltonian.

3. Plot the first four (or more) energy levels $E_n(\lambda)$ versus λ over the range $0 \leq \lambda \leq 1$. Plot also the spacings between the levels $\Delta E(\lambda) = E_{n+1}(\lambda) - E_n(\lambda)$. Make sure to use a basis size N (much) larger than the desired number of lowest eigenvalues.

4. Check the convergence of the method with respect to the basis size N by plotting one of the lowest (or more) energy eigenvalues $E_n(N)$ for $\lambda = 1$ versus the basis size N. Alternatively, to demonstrate the convergence more clearly, you can also plot the differences between two consecutive estimates $\epsilon_n = E_n(N) - E_n(N+2)$ versus N.

5. Plot and compare compare the first two (or more) eigenfunctions $\psi_n(x)$ for the harmonic oscillator with $\lambda = 0$ to the eigenfunctions for the anharmonic oscillator with $\lambda = 1$.