Assignment 2

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(Dated: 16 May 2017)

In the second assignment, I computationally create the position operator in the second order and quartic on python, and from there create an array of $(N+1) \times (N+1)$ matrix. With this, I computationally solve the anharmonic eigenvalue problem for the first four energy levels with $N = 600$ which would converge to an approximate form of the true eigenvalues. The results I received for E_0, E_1, E_2, E_3 with the constant $\lambda = 1$ are 0.80377065, 2.73789227, 5.17929169, 7.94240398 with percent errors to the real values of 0%, 0%, 0%, and 1.26×10^{-7}% respectively. Next, I plotted the anharmonic in three different ways: the first four energy levels versus the constant λ; the lowest energy eigenvalues versus basis size N with the constant $\lambda = 1$; and comparing the eigenfunctions for the harmonic oscillator with $\lambda = 0$ to the eigenfunctions for the anharmonic oscillator with $\lambda = 1$.

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I. INTRODUCTION

The quantum harmonic oscillator is defined by the unperturbed Hamiltonian having the form of a second-order position and momentum operator such that: (annotate class pdf)

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

The position as well as the momentum operator can be defined by linear algebra of a raising operator $\hat{a}$ and a lowering operator $\hat{a}^\dagger$ where: (annotate book)

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

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

This means that the Hamiltonian can be written in terms of the raising and lowering operator such that: (annotate book)

$$\hat{H}_0 = \hat{a}\hat{a}^\dagger + \frac{1}{2}\hat{I}, \tag{4}$$

where $\hat{I}$ is the identity matrix.

When a wavefunction such as ψ_m acts on the raising and lowering operators, then: (annotate book)

$$\hat{a}|\psi_m\rangle = \hat{a}|m\rangle = \sqrt{m+1}|m+1\rangle \tag{5}$$

$$\hat{a}^\dagger|\psi_m\rangle = \hat{a}^\dagger|m\rangle = \sqrt{m}|m-1\rangle. \tag{6}$$

Then, with $\langle n|$ acting on both of these operators, the results are:(annotate book)

$$\langle n|\hat{a}|m\rangle = \sqrt{m+1}\delta_{n,m+1} \tag{7}$$

$$\langle n|\hat{a}^\dagger|m\rangle = \sqrt{m}\delta_{n,m-1}. \tag{8}$$

Now, when they act on the Hamiltonian, the result is:(annotate book)

$$\langle n|\hat{H}_0|m\rangle = (m + \frac{1}{2})\delta_{n,m}, \tag{9}$$

which would give you the energy eigenvalues E_m.

II. THE SECOND ORDER AND QUARTIC OPERATORS

For the second order operator of a harmonic oscillator, and by the definition that the raising and lowering operators do not commute, then:

$$\langle n|\hat{x}^2|m\rangle = \langle n| \tag{10}$$

III. ANHARMONIC OSCILLATOR EIGENVALUE PROBLEM

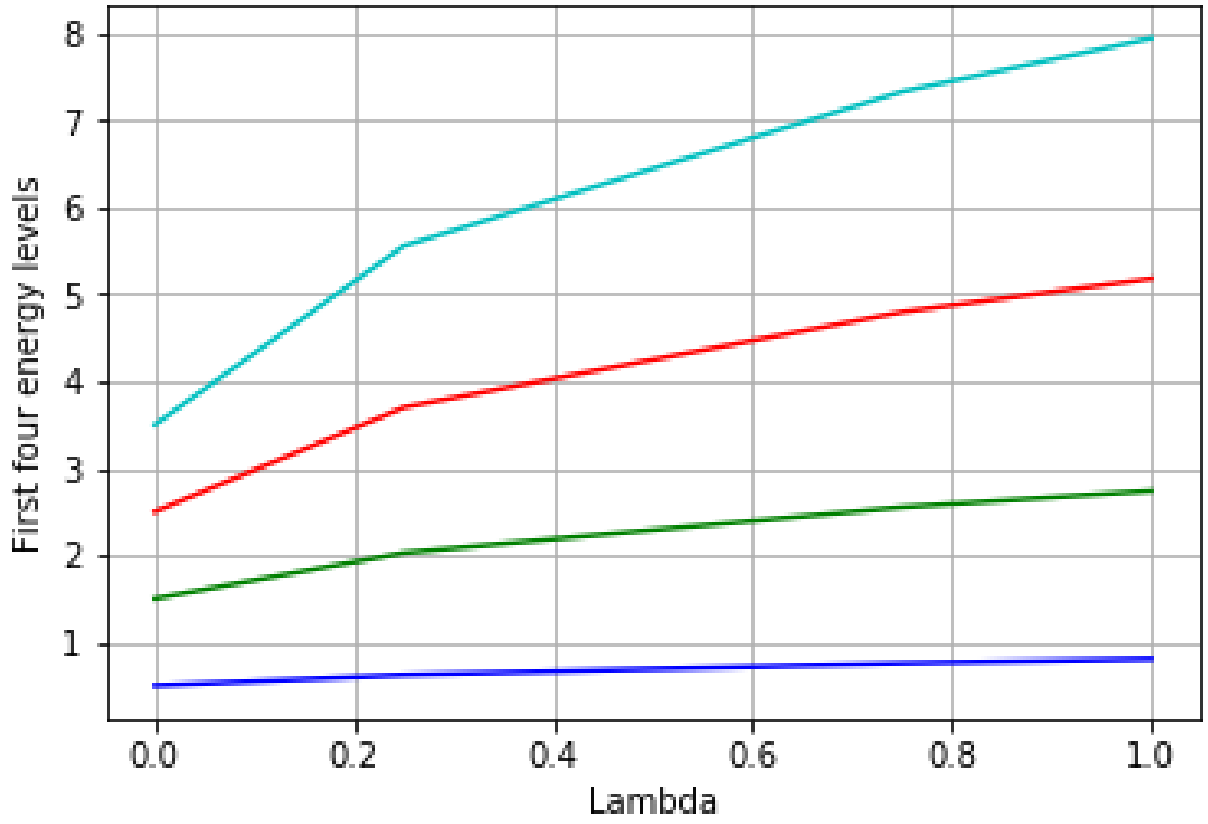
I created a Hamiltonian which consists of the original Hamiltonian as well as the quartic/constant-λ, and created a matrix element. This would help me to find the eigenvalues of the problem, and to find the eigenvalues more accurately, I used a special scipy package which would extract the small eigenvalues and not the larger ones. From there I received my eigenvalues of 0.80377065, 2.73789227, 5.17929169, and 7.94240398 while the real values are 0.80377065, 2.73789227, 5.17929169, and 7.94240399 which gave me a percent errors of 0%, 0%, 0%, and 1.26×10^{-7}% respectively. The full description on how it works is shown in the ipynb file.

IV. PLOTTING THE FIRST FOUR $E_n(\lambda)$ VERSUS λ

When I plot the energy levels versus the constant lambda over the range $0 \leq \lambda \geq$, I do not include the plot spacings between the levels $\Delta E(\lambda) = E_{n+1}(\lambda) - E_n(\lambda)$. When setting the parameters, I used numpy, pylab, and matplotlib. As

I set $N = 600$ to get the accurate values of the energy eigenvalues while I vary the constant λ's and the anharmonic's in order. For the λ's, I used four values since it would not crash python and for it to compute faster, and those values are 0, 0.25, 0.75, and 1 which would be used as well to create an x-array.

For the anharmonic's, I used those four λ's to create four anharmonics and created a matrix elements of those eigenvalues. To show how each of the energy levels changes from different values of λ, I would extract the first four eigenvalues that are affected by the different lambda's such as E_0, E_1, E_2, and E_3. I would individually put each of those energy levels in a y-arrays. Then, I would plot each of those y-arrays with the x-array and achieved of plotting the first four energy levels as shown below:

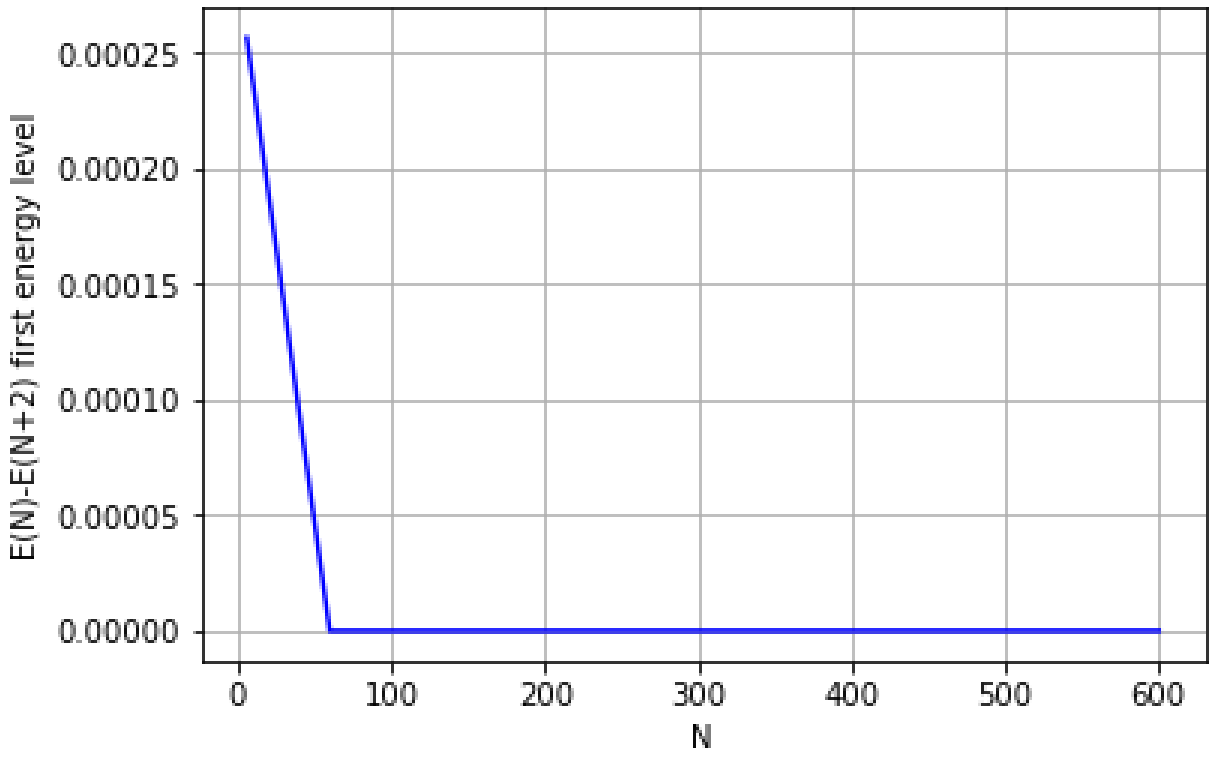


This graph shows that as the higher the constant λ is, the more the anharmonic energy levels increases.

V. CONVERGENCE OF THE METHOD

The next step is to plot the lowest energy eigenvalues for $\lambda = 1$ versus the basis size N, and the lowest energy eigenvalues I have chosen was E_0. The procedure is the same as the previous section only this time λ was held constant as I vary both the basis size as well as the anharmonics. I constructed ten anharmonics for $E_0(N)$ as well as ten $E_0(N+2)$,

subtracted the two and plug it made them into y-arrays. From there is where I plotted the between two consecutive estimates versus the basis size which is shown below:



From here it shows that as the basis size increases, then the energy levels become more and more accurate to the true values.