Midterm 4: Investigation of Bound States in 1D Harmonic Oscillator with Given Potential

Computational Physics - Phys 562

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Abstract

No abstract

1 Introduction

Analysis of a 1D harmonic oscillator can give us good insight into the underlying physics of certain systems as well as the effects of the different alternate parameters introduce into the basis for the total energy. We will look at the effects of the establishing a new potential (V) for this basis, from here a new computationally consistent Hamiltonian can be formed with addition of the (what will have to be) calculated matrix for kinetic.

$$\hat{T} + \hat{V} = \hat{H} \tag{1}$$

Where V is defined to be,

$$V(x) = -\frac{10}{|i + x|} \tag{2}$$

This Hamiltonian matrix contains the measurement of the total energy for this system, from which the eigenvalues and eigenstates can be expected. The importance these necessary functions will be discussed further in the report

as they relate to the changing parameters. When this is done bound states for this system are distinguished apart from the free states, giving a physical meaning to the local neighbor of the particle or particle in the researched system. This is not a new challenge as we a previously perform parts of the code to be used. The complexity will arise in the perform the model of the new potential and correctly computing its behavior. Strong understanding of quantum mechanics is needed to grasp the subtle meaning of each of the numerical methods used herein, as well as working knowledge of the Fortran environment.

2 The Math

Beginning with our knowledge of the total energy for a 1-D oscillating system;

$$\hat{T_n}|\psi\rangle + \hat{U}|\psi\rangle = \hat{E_n}|\psi_n\rangle \tag{3}$$

Where $|\psi\rangle$ used in class previously as,

$$\psi_n(x) = \frac{1}{\sqrt{2^n\, n!}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot e^{-\frac{m\omega x^2}{2\hbar}} \cdot H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \tag{4}$$

and $\hat{E_n}$ as

$$\hat{E_n} = \left(n + \frac{1}{2}\right)\hbar\omega \tag{5}$$

Finally the operator $\hat{U}$ as

$$\hat{U} = \frac{1}{2}m\omega^2\hat{x^2} \tag{6}$$

To find the kinetic energy we must perform some rearrangement,

$$\hat{T_n}|\psi\rangle = \hat{E_n}|\psi_n\rangle - \hat{U}|\psi\rangle \tag{7}$$

Using the following operations to create matrices,

$$A_{m,n} = \langle\psi_n|\hat{A}|\psi_n\rangle \tag{8}$$

$$\langle\psi_i|\psi_j\rangle = \int_{-\infty}^{\infty} \psi_i^*(x)\,\psi_j(x)\,dx = I \tag{9}$$

We can write the following,

$$\langle\psi_n|\hat{T}|\psi_n\rangle = \langle\psi_n|\hat{E}_n|\psi_n\rangle - \langle\psi_n|\hat{U}|\psi_n\rangle \tag{10}$$

Note integration on the E_n does not need to be perform has it has no reliance on the x parameter. We can finally write,

$$T_{m,n} = \int_a^b \psi_m^*[(n+\frac{1}{2})\hbar\omega]\psi_n dx - \int_a^b \psi_m^*[\frac{1}{2}m\omega^2\hat{x}^2]\psi_n dx \tag{11}$$

Which can be simplified to,

$$T_{m,n} = E_n - \frac{1}{2}m\omega^2 \int_a^b \psi_m^*\hat{x}^2\psi_n dx \tag{12}$$

Establishing E as a matrix and evaluating the integral,

$$T_{m,n} = E_{m,n} + U_{m,n} \tag{13}$$

From this we are required to calculate a new Hamiltonian utilizing the given potential $V(x) = -\frac{10}{|i+x|}$ by,

$$H_{m,n} = T_{m,n} + V_{m,n} \tag{14}$$

As stated above the iterated eigenvalues and eigenstates can be comprised from the resulting hamiltonian.

3 The Code

To begin we initiated the code with a module, to house all variables indicating wether they were to be used as real, integer or array values. Some components of the early declarations are to be used in external subroutine for later calculations of the certain elements. File named, `d01b.f95` have been added to the mother directory labeled `code` for this purpose. External functions are created for computations of qualities that will be called into the main routine such as the psi functions that will iterate an integer number of times as needed, the potential operator $(\hat{U})$ is really just an external function as well and finally a function for the new potential $V(x) = -\frac{10}{|i+x|}$. The main routine begins with the integration for the E matrix is not needed, so to put this into the code E was removed and done explicitly through a series of

nested do loops entered diagonally as the energies of the harmonic oscillator. The wave integral is understood to be the identity matrix and ignored. The next step is to utilize the subroutine `d01bcf.f95`, this is used to integrate the first potential function U with the psi functions (calculated below) using Guass-Legrendre. It should be noted that this is done simultaneously for the new potential (V) in the same loop. Saving this to matrix elements we have all the necessary components to perform the matrix arithmetic (12) (13) to achieve the new hamiltonian. We have created a shifted duplicate hamiltonian, so that the then called `dsyev` can analytically produce the eigenvalues and eigenstates. We have cut off the positive eigenvalues, as these are outside the area of bound value and correspond to "free values" outside of the potential well.

4 The Results

As indicated by the test sheet the values for omega have been manually irritated, as discussed in class it has been determined that ω=1 provides the best estimation for the lowest eigenvalues. Completely removing the positive values allows us to analyze only values that remain in the potential well of the function, with this information we can recognize that these bound states are the local regions were the particle or particles depending on the system are expected to be found. Below we can see the eigenvalues (eigen-energies) and the column vector of the associated eigenstates for n to 10. As I have only given ten values, to comply with the test parameter for the dimension `ndim` of 30, we can manually change this in the module

1	-8.6473696457981344
2	-6.3682627596826960
3	-4.8037174853406475
4	-3.7027145474319343
5	-2.9186802374149203
6	-2.3092318003945116
7	-1.7600582655607726
8	-0.77760076286157809
9	$-7.9663132970126421E-002$
10	$[positive]$

Table 1: Eigenvalues for $\omega = 1$

With the associated eigen-vectors being shown (below) here columns 1-9,

$$\begin{bmatrix} 0.961 & 0.000 & -0.275 & 0.000 & -0.036 & -0.000 & 0.010 & 0.000 & -0.004 \\ -0.000 & 0.944 & 0.000 & 0.312 & -0.000 & 0.098 & -0.000 & -0.040 & 0.000 \\ -0.253 & 0.000 & -0.922 & 0.000 & 0.235 & 0.000 & -0.158 & -0.000 & 0.077 \\ 0.000 & -0.294 & 0.000 & 0.935 & -0.000 & -0.075 & -0.000 & 0.161 & 0.000 \\ 0.101 & -0.000 & 0.225 & -0.000 & 0.943 & 0.000 & -0.149 & 0.000 & -0.124 \\ -0.000 & 0.133 & -0.000 & -0.074 & 0.000 & -0.918 & -0.000 & 0.333 & 0.000 \\ -0.046 & 0.000 & -0.140 & 0.000 & 0.121 & -0.000 & 0.844 & 0.000 & -0.489 \\ 0.000 & -0.060 & -0.000 & 0.147 & 0.000 & -0.273 & -0.000 & -0.868 & -0.000 \\ 0.023 & -0.000 & 0.056 & 0.000 & 0.202 & 0.000 & 0.373 & -0.000 & 0.779 \end{bmatrix}$$

5 The Results

In conclusion, each column above is comprised of the set of eigenvectors corresponding to the numerated eigen-energies (Table 1). It is important to mention the 10th column has been left out for clarity due to its associated positive eigenvalues. Once again we report the negative values only as they are the bound states (of new Hamiltonian for the V potential). Combining the eigenvalues with the eigenstates gives better representation of the placement of each wave and its energy within the potential well.

References

[1] Z. Papp and A. Bill, *Computational Physics Lecture Notes*, California State University Long Beach.