Jacobi_Algorithm

December 18, 2018

1 Using the Jacobi Algorithm to compute the Eigenvalues and Eigenvectors for Quantum Systems

1.1 Numerical Solution Functions

In [7]:
```
import numpy as np
from numpy.linalg import norm
from scipy.stats import unitary_group

def off(M):
    rows = M.shape[0]
    columns = M.shape[1]
    sum0 = 0
    for i in range(rows):
        for k in range(columns):
            if(i != k):
                sum0 += abs(M[i, k])**2
    return sum0**(1/2)


def splitMatrix(M):
    return M.real, M.imag


#The numerical method used to diagonalize a matrix
#p and q are integers limited by: 1 <= p < q <= n
def jacobiRotation(M, p, q):
    c = 0
    s = 0
    if M[p, q] != 0:
        tau = (M[q, q] - M[p, p]) / (2 * M[p, q])
        if tau >= 0:
            t = 1/(tau + (1 + tau**2)**(1/2))
        else:
            t = 1/(tau - (1 + tau**2)**(1/2))
        c = 1/((1 + t**2)**(1/2))
        s = t * c
```

```
    else:
        c = 1
        s = 0
    J = np.identity(M.shape[0])
    J[p, p] = c
    J[p, q] = s
    J[q, p] = -s
    J[q, q] = c
    return J


def real_eigen(M, tolerance):
    n = M.shape[0]
    R = np.identity(n)
    delta = tolerance*(norm(M))
    while off(M) > delta:
        for p in range(0, n-1):
            for q in range(p + 1, n):
                J = jacobiRotation(M, p, q)
                M = (J.transpose().dot(M)).dot(J)
                R = R.dot(J)
    d = np.array([M[i, i] for i in range(n)])
    return d, R

def complex_eigen(H, tolerance):
    S, A = splitMatrix(H)

    O1 = np.concatenate((S, A), axis=0)
    O2 = np.concatenate((-A, S), axis=0)
    O = np.concatenate((O1, O2), axis=1)

    dd, R = real_eigen(O, tolerance)

    rRows = R.shape[0]
    U0 = np.zeros((int(rRows / 2), int(rRows)), dtype=complex)
    for i in range(0, rRows):
        U0[:, i] = R[:int(rRows/2), i] + (R[int(rRows/2):, i]*1j)

    index = np.argsort(dd)
    dd = dd[index]
    U0 = U0[:, index]

    d = np.array([dd[i] for i in range(0, len(dd), 2)])
    U = np.zeros((int(rRows / 2), int(rRows/2)), dtype=complex)

    for i in range(0, rRows,2):
        if norm(U0[:,i] > U0[:,i+1]):
            U[:,int(i/2)] = U0[:,i]
```

```
        else:
            U[:,int(i/2)] = U0[:,i+1]
    return d, U

def hermitian_eigensystem(H, tolerance):

    """ Solves for the eigenvalues and eigenvectors of a hermitian matrix

    Args:
        H: Hermitian matrix for which we want to compute eigenvalues and eigenvectors

        tolerance: A number that sets the tolerance for the accuracy of the computatio
        is multiplied by the norm of the matrix H to obtain a number delta.  The algor
        applies (via similarity transformation) Jacobi rotations to the matrix H until
        squares of the off-diagonal elements are less than delta.



    Returns:
        d: Numpy array containing eigenvalues of H in non-decreasing order

        U: A 2d numpy array whose columns are the eigenvectors corresponding to the co
        eigenvalues.


    Checks you might need to do:

        H * U[:,k] = d[k] *U[:,k]      k=0,1,2,...,(n-1)

        d[0] <= d[1] <= ... <= d[n-1]     (where n is the dimension of H)

        np.transpose(U) * U = U * np.transpose(U) = np.eye(n)

    """

    d, U = complex_eigen(H, tolerance)
    index = np.argsort(d)
    d = d[index]
    U = U[:, index]


    return d, U

#Creates a Hermitian matrix of size n x n and returns the matrix along with its exact
def createHermitian(n):
    p = unitary_group.rvs(n)
    b = np.random.randint(-2000,2000,size=(n))
    arr = np.diag(b)
```

```
        herm = np.matrix(p).dot(arr).dot(np.matrix(p).H)
        diag = np.diag(herm).real
        np.fill_diagonal(herm,diag)
        return herm, b
```

1.1.1 Numerical Solution Tests

The numerical solutions are tested by first comparing the computed eigenvalues to the exact eigenvalues (Matrices with known eigenvalues are used).

Next, the accuracy of the numerical solution is tested by ensuring the following equation holds true:

$$Av = \lambda v \tag{1}$$

where A is the hermitian matrix, v is the eigenvector, and λ is the corresponding eigenvalue.

Lastly, the following equation is checked to ensure that the numerical solution is accurate:

$$U^{\dagger}U = UU^{\dagger} \tag{2}$$

where U is the computed eigenvector matrix.

The accuracy of these tests should be within the tolerance specified when calling the hermitian_eigensystem function. In this case it is 0.01.

```
In [8]: n = 2
        herm, b = createHermitian(n)
        tolerance = 0.1
        d, U = hermitian_eigensystem(herm, 0.01)

        print("FOR HERMITIAN MATRIX SIZE: ", n)
        print("Eigenvalues from createHermitian function:", b)
        print("Eigenvalues from numerical solution:", d)
        print("\n")

        for i in range(n):
            print("Hermitian matrix * Eigenvector {0}: ".format(i + 1), np.array(herm.dot(U[:,
            print("Eigenvalue {0} * Eigenvector {0}:     ".format(i + 1), d[i] * U[:, i])
            print("\n")


        print("Hermitian of U * U: ", "\n", (U.conj().transpose().dot(U)))
        print("U * Hermitian of U: ", "\n", U.dot(U.conj().transpose()))
```

```
FOR HERMITIAN MATRIX SIZE:  2
Eigenvalues from createHermitian function: [-363 1178]
Eigenvalues from numerical solution: [-363. 1178.]


Hermitian matrix * Eigenvector 1:  [-322.1528 +34.7693j  -36.3207-159.5572j]
Eigenvalue 1 * Eigenvector 1:      [-322.1528 +34.7693j  -36.3207-159.5572j]
```

```
Hermitian matrix * Eigenvector 2:  [ -35.3833+529.8574j 1050.22   -52.1641j]
Eigenvalue 2 * Eigenvector 2:      [ -35.3833+529.8574j 1050.22   -52.1641j]


Hermitian of U * U:
 [[ 1.0000e+00-5.5320e-18j -6.9389e-17-5.5511e-17j]
 [-6.9389e-17+0.0000e+00j  1.0000e+00+3.0014e-18j]]
U * Hermitian of U:
 [[ 1.0000e+00+0.0000e+00j -4.8572e-17-2.2204e-16j]
 [-4.8572e-17+2.2204e-16j  1.0000e+00+0.0000e+00j]]
```

Slight variations of the tests are then ran for multiple matrices of different sizes.

```
In [9]: nums = [3, 5, 10, 15, 20, 30]
        %precision 4
        for n in nums:
            herm, b = createHermitian(n)
            tolerance = 0.001
            d, U = hermitian_eigensystem(herm, tolerance)

            print("FOR HERMITIAN MATRIX SIZE: ", n)
            print("Eigenvalues from createHermitian function:", "\n", b)
            print("Eigenvalues from numerical solution:", "\n", d)
            print("\n")

            for i in range(n):
                norm1 = np.linalg.norm(np.array(herm.dot(U[:,i])).reshape(n,) - d[i] * U[:, i]
                norm2 = np.linalg.norm(np.array(herm.dot(U[:,i])).reshape(n,))
                print("Standardized Norm of (Hermitian matrix * Eigenvector {0}) - (Eigenvalue


            print("\n")
            print("Norm of off-diagnoal elements of Hermitian of U * U: ", "\n", off(U.conj().
            print("Norm of off-diagnoal elements of U * Hermitian of U: ", "\n", off(U.dot(U.co
```

```
FOR HERMITIAN MATRIX SIZE:  3
Eigenvalues from createHermitian function:
 [  863  1283 -1320]
Eigenvalues from numerical solution:
 [-1320.   863.  1283.]


Standardized Norm of (Hermitian matrix * Eigenvector 1) - (Eigenvalue 1 * Eigenvector 1):
 6.0297600054270875e-06
Standardized Norm of (Hermitian matrix * Eigenvector 2) - (Eigenvalue 2 * Eigenvector 2):
```

```
 4.116071455196522e-07
Standardized Norm of (Hermitian matrix * Eigenvector 3) - (Eigenvalue 3 * Eigenvector 3):
 5.700736441668461e-06


Norm of off-diagnoal elements of Hermitian of U * U:
 2.831451674637223e-06
Norm of off-diagnoal elements of U * Hermitian of U:
 2.6666513371484775e-06

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FOR HERMITIAN MATRIX SIZE:  5
Eigenvalues from createHermitian function:
 [ 1294  -232  -580 -1059  1652]
Eigenvalues from numerical solution:
 [-1059.      -580.      -232.      1294.      1651.9999]


Standardized Norm of (Hermitian matrix * Eigenvector 1) - (Eigenvalue 1 * Eigenvector 1):
 8.008776085572285e-05
Standardized Norm of (Hermitian matrix * Eigenvector 2) - (Eigenvalue 2 * Eigenvector 2):
 6.7941789836144e-07
Standardized Norm of (Hermitian matrix * Eigenvector 3) - (Eigenvalue 3 * Eigenvector 3):
 2.1935585548783933e-06
Standardized Norm of (Hermitian matrix * Eigenvector 4) - (Eigenvalue 4 * Eigenvector 4):
 4.191906192108044e-08
Standardized Norm of (Hermitian matrix * Eigenvector 5) - (Eigenvalue 5 * Eigenvector 5):
 0.00024440752185097246


Norm of off-diagnoal elements of Hermitian of U * U:
 0.0004250166677504974
Norm of off-diagnoal elements of U * Hermitian of U:
 0.000397701889774663

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FOR HERMITIAN MATRIX SIZE:  10
Eigenvalues from createHermitian function:
 [ -201    -6  1928   589 -1774  1633 -1596  -763  1995  -917]
Eigenvalues from numerical solution:
 [-1774. -1596.  -917.  -763.  -201.    -6.   589.  1633.  1928.  1995.]


Standardized Norm of (Hermitian matrix * Eigenvector 1) - (Eigenvalue 1 * Eigenvector 1):
 7.080507485261634e-07
Standardized Norm of (Hermitian matrix * Eigenvector 2) - (Eigenvalue 2 * Eigenvector 2):
```

```
 6.067204234354772e-08
Standardized Norm of (Hermitian matrix * Eigenvector 3) - (Eigenvalue 3 * Eigenvector 3):
 5.384540012679298e-06
Standardized Norm of (Hermitian matrix * Eigenvector 4) - (Eigenvalue 4 * Eigenvector 4):
 4.3065188403098437e-07
Standardized Norm of (Hermitian matrix * Eigenvector 5) - (Eigenvalue 5 * Eigenvector 5):
 3.0311178218989714e-07
Standardized Norm of (Hermitian matrix * Eigenvector 6) - (Eigenvalue 6 * Eigenvector 6):
 2.3033933893549735e-07
Standardized Norm of (Hermitian matrix * Eigenvector 7) - (Eigenvalue 7 * Eigenvector 7):
 1.1257470891626755e-09
Standardized Norm of (Hermitian matrix * Eigenvector 8) - (Eigenvalue 8 * Eigenvector 8):
 1.4558811585096854e-07
Standardized Norm of (Hermitian matrix * Eigenvector 9) - (Eigenvalue 9 * Eigenvector 9):
 2.833669146071198e-06
Standardized Norm of (Hermitian matrix * Eigenvector 10) - (Eigenvalue 10 * Eigenvector 10):
 5.150656909631893e-05


Norm of off-diagnoal elements of Hermitian of U * U:
 4.805662122788937e-05
Norm of off-diagnoal elements of U * Hermitian of U:
 4.640559404448336e-05

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FOR HERMITIAN MATRIX SIZE:  15
Eigenvalues from createHermitian function:
 [ 1439  1749  -224   326    85  1250   120  1833  -212  1795    78 -1463
 -1012  -801  -452]
Eigenvalues from numerical solution:
 [-1463.     -1012.      -801.      -452.      -224.0002  -212.
    78.        85.       120.       326.      1250.      1439.
  1749.      1795.      1833.    ]


Standardized Norm of (Hermitian matrix * Eigenvector 1) - (Eigenvalue 1 * Eigenvector 1):
 2.6094080144594608e-06
Standardized Norm of (Hermitian matrix * Eigenvector 2) - (Eigenvalue 2 * Eigenvector 2):
 8.60070007323133e-05
Standardized Norm of (Hermitian matrix * Eigenvector 3) - (Eigenvalue 3 * Eigenvector 3):
 1.8809305397301454e-07
Standardized Norm of (Hermitian matrix * Eigenvector 4) - (Eigenvalue 4 * Eigenvector 4):
 1.0119747056445961e-06
Standardized Norm of (Hermitian matrix * Eigenvector 5) - (Eigenvalue 5 * Eigenvector 5):
 0.0022027837363084476
Standardized Norm of (Hermitian matrix * Eigenvector 6) - (Eigenvalue 6 * Eigenvector 6):
 2.6364734381242033e-05
```

```
Standardized Norm of (Hermitian matrix * Eigenvector 7) - (Eigenvalue 7 * Eigenvector 7):
 0.00011501363232998525
Standardized Norm of (Hermitian matrix * Eigenvector 8) - (Eigenvalue 8 * Eigenvector 8):
 3.409214041093725e-06
Standardized Norm of (Hermitian matrix * Eigenvector 9) - (Eigenvalue 9 * Eigenvector 9):
 4.539448496935177e-05
Standardized Norm of (Hermitian matrix * Eigenvector 10) - (Eigenvalue 10 * Eigenvector 10):
 9.463592337538574e-06
Standardized Norm of (Hermitian matrix * Eigenvector 11) - (Eigenvalue 11 * Eigenvector 11):
 4.812146856741937e-07
Standardized Norm of (Hermitian matrix * Eigenvector 12) - (Eigenvalue 12 * Eigenvector 12):
 1.7177767908947583e-05
Standardized Norm of (Hermitian matrix * Eigenvector 13) - (Eigenvalue 13 * Eigenvector 13):
 2.7052162165307967e-05
Standardized Norm of (Hermitian matrix * Eigenvector 14) - (Eigenvalue 14 * Eigenvector 14):
 0.00015988657516398635
Standardized Norm of (Hermitian matrix * Eigenvector 15) - (Eigenvalue 15 * Eigenvector 15):
 8.326803931784259e-05


Norm of off-diagnoal elements of Hermitian of U * U:
 0.0009887585204033345
Norm of off-diagnoal elements of U * Hermitian of U:
 0.0009807629980607936

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FOR HERMITIAN MATRIX SIZE:  20
Eigenvalues from createHermitian function:
 [ 1358 -1147 -1201  1292 -1800  -522  -862  1590   849  -931  1130   603
   245 -1886  -500 -1840   664  -642   572   603]
Eigenvalues from numerical solution:
 [-1885.9998 -1840.0135 -1800.0001 -1201.     -1147.      -931.
  -861.9998  -642.      -522.0002  -500.0006   245.       571.9997
   602.9999   603.       663.9997   848.9999  1129.9967  1291.9991
  1357.9996  1589.9985]


Standardized Norm of (Hermitian matrix * Eigenvector 1) - (Eigenvalue 1 * Eigenvector 1):
 7.37943119264631e-05
Standardized Norm of (Hermitian matrix * Eigenvector 2) - (Eigenvalue 2 * Eigenvector 2):
 0.00198923604273857
Standardized Norm of (Hermitian matrix * Eigenvector 3) - (Eigenvalue 3 * Eigenvector 3):
 0.0001188639775078139
Standardized Norm of (Hermitian matrix * Eigenvector 4) - (Eigenvalue 4 * Eigenvector 4):
 5.642921780846332e-05
Standardized Norm of (Hermitian matrix * Eigenvector 5) - (Eigenvalue 5 * Eigenvector 5):
 0.0005562411314495131
```

```
Standardized Norm of (Hermitian matrix * Eigenvector 6) - (Eigenvalue 6 * Eigenvector 6):
 0.00011264082768862287
Standardized Norm of (Hermitian matrix * Eigenvector 7) - (Eigenvalue 7 * Eigenvector 7):
 0.000496739206701756
Standardized Norm of (Hermitian matrix * Eigenvector 8) - (Eigenvalue 8 * Eigenvector 8):
 1.120482285694032e-06
Standardized Norm of (Hermitian matrix * Eigenvector 9) - (Eigenvalue 9 * Eigenvector 9):
 0.0010356617307860486
Standardized Norm of (Hermitian matrix * Eigenvector 10) - (Eigenvalue 10 * Eigenvector 10):
 0.0014645747016552545
Standardized Norm of (Hermitian matrix * Eigenvector 11) - (Eigenvalue 11 * Eigenvector 11):
 0.0002571665055092669
Standardized Norm of (Hermitian matrix * Eigenvector 12) - (Eigenvalue 12 * Eigenvector 12):
 0.0011387775361714663
Standardized Norm of (Hermitian matrix * Eigenvector 13) - (Eigenvalue 13 * Eigenvector 13):
 0.0005588308866080197
Standardized Norm of (Hermitian matrix * Eigenvector 14) - (Eigenvalue 14 * Eigenvector 14):
 5.589135582219118e-05
Standardized Norm of (Hermitian matrix * Eigenvector 15) - (Eigenvalue 15 * Eigenvector 15):
 0.0010799171229837943
Standardized Norm of (Hermitian matrix * Eigenvector 16) - (Eigenvalue 16 * Eigenvector 16):
 0.0003072146704707869
Standardized Norm of (Hermitian matrix * Eigenvector 17) - (Eigenvalue 17 * Eigenvector 17):
 0.0028630158102865275
Standardized Norm of (Hermitian matrix * Eigenvector 18) - (Eigenvalue 18 * Eigenvector 18):
 0.0013077987866164692
Standardized Norm of (Hermitian matrix * Eigenvector 19) - (Eigenvalue 19 * Eigenvector 19):
 0.0008175662360009883
Standardized Norm of (Hermitian matrix * Eigenvector 20) - (Eigenvalue 20 * Eigenvector 20):
 0.0011366754612975756


Norm of off-diagnoal elements of Hermitian of U * U:
 0.40787361920377296
Norm of off-diagnoal elements of U * Hermitian of U:
 0.3965624177692377

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FOR HERMITIAN MATRIX SIZE:  30
Eigenvalues from createHermitian function:
 [-1566 -1851   524 -1854  1951    11 -1858  1442  -609  1630 -1791   323
 -1593 -1636  1846  1172  1148   578  1950   301  -790  -582  1785  -451
  -577 -1594  -533  1211   322    28]
Eigenvalues from numerical solution:
 [-1857.9734 -1854.0025 -1851.0774 -1791.0059 -1636.0073 -1594.0048
 -1593.0165 -1566.      -790.      -609.      -582.      -577.
  -533.      -451.        11.        28.       301.       322.
```

```
  323.        524.        578.       1148.       1172.       1211.
 1442.       1629.9994   1785.       1846.       1949.9997   1950.9941]
```

```
Standardized Norm of (Hermitian matrix * Eigenvector 1) - (Eigenvalue 1 * Eigenvector 1):
 0.0017540070999773473
Standardized Norm of (Hermitian matrix * Eigenvector 2) - (Eigenvalue 2 * Eigenvector 2):
 0.00024097716517337397
Standardized Norm of (Hermitian matrix * Eigenvector 3) - (Eigenvalue 3 * Eigenvector 3):
 0.0005004875280560246
Standardized Norm of (Hermitian matrix * Eigenvector 4) - (Eigenvalue 4 * Eigenvector 4):
 0.0008982639548848178
Standardized Norm of (Hermitian matrix * Eigenvector 5) - (Eigenvalue 5 * Eigenvector 5):
 0.0012858026604550628
Standardized Norm of (Hermitian matrix * Eigenvector 6) - (Eigenvalue 6 * Eigenvector 6):
 0.0008841383256327122
Standardized Norm of (Hermitian matrix * Eigenvector 7) - (Eigenvalue 7 * Eigenvector 7):
 0.0015578446893683268
Standardized Norm of (Hermitian matrix * Eigenvector 8) - (Eigenvalue 8 * Eigenvector 8):
 7.61136327386145e-05
Standardized Norm of (Hermitian matrix * Eigenvector 9) - (Eigenvalue 9 * Eigenvector 9):
 7.760299014566338e-05
Standardized Norm of (Hermitian matrix * Eigenvector 10) - (Eigenvalue 10 * Eigenvector 10):
 6.278474608744947e-06
Standardized Norm of (Hermitian matrix * Eigenvector 11) - (Eigenvalue 11 * Eigenvector 11):
 7.83462222814601e-05
Standardized Norm of (Hermitian matrix * Eigenvector 12) - (Eigenvalue 12 * Eigenvector 12):
 7.307257939328021e-07
Standardized Norm of (Hermitian matrix * Eigenvector 13) - (Eigenvalue 13 * Eigenvector 13):
 1.2135361873081042e-06
Standardized Norm of (Hermitian matrix * Eigenvector 14) - (Eigenvalue 14 * Eigenvector 14):
 5.42290477132897e-07
Standardized Norm of (Hermitian matrix * Eigenvector 15) - (Eigenvalue 15 * Eigenvector 15):
 1.8836879205732955e-06
Standardized Norm of (Hermitian matrix * Eigenvector 16) - (Eigenvalue 16 * Eigenvector 16):
 0.0010183246739226218
Standardized Norm of (Hermitian matrix * Eigenvector 17) - (Eigenvalue 17 * Eigenvector 17):
 1.014063486031068e-08
Standardized Norm of (Hermitian matrix * Eigenvector 18) - (Eigenvalue 18 * Eigenvector 18):
 1.8441453800571177e-07
Standardized Norm of (Hermitian matrix * Eigenvector 19) - (Eigenvalue 19 * Eigenvector 19):
 6.373077862022432e-07
Standardized Norm of (Hermitian matrix * Eigenvector 20) - (Eigenvalue 20 * Eigenvector 20):
 4.436250116411622e-07
Standardized Norm of (Hermitian matrix * Eigenvector 21) - (Eigenvalue 21 * Eigenvector 21):
 5.00084408848551e-08
Standardized Norm of (Hermitian matrix * Eigenvector 22) - (Eigenvalue 22 * Eigenvector 22):
 4.2139294088525475e-06
```

```
Standardized Norm of (Hermitian matrix * Eigenvector 23) - (Eigenvalue 23 * Eigenvector 23):
 5.930541975706837e-05
Standardized Norm of (Hermitian matrix * Eigenvector 24) - (Eigenvalue 24 * Eigenvector 24):
 0.0002965067947524356
Standardized Norm of (Hermitian matrix * Eigenvector 25) - (Eigenvalue 25 * Eigenvector 25):
 3.7723348265549304e-05
Standardized Norm of (Hermitian matrix * Eigenvector 26) - (Eigenvalue 26 * Eigenvector 26):
 0.0008784475836014979
Standardized Norm of (Hermitian matrix * Eigenvector 27) - (Eigenvalue 27 * Eigenvector 27):
 8.714663985434631e-05
Standardized Norm of (Hermitian matrix * Eigenvector 28) - (Eigenvalue 28 * Eigenvector 28):
 2.131759469490622e-05
Standardized Norm of (Hermitian matrix * Eigenvector 29) - (Eigenvalue 29 * Eigenvector 29):
 0.0004974695111783754
Standardized Norm of (Hermitian matrix * Eigenvector 30) - (Eigenvalue 30 * Eigenvector 30):
 0.0023932221257416597


Norm of off-diagnoal elements of Hermitian of U * U:
 0.23188054679491213
Norm of off-diagnoal elements of U * Hermitian of U:
 0.22740240015250648

 ---------------------------------------------
```

1.2 Analyzing the Anharmonic Oscillator

The Hamiltonian that governs the anharmonic oscillator is:

$$\hat{H}_\lambda = \hat{H}_0 + \lambda \hat{x}^4 \tag{3}$$

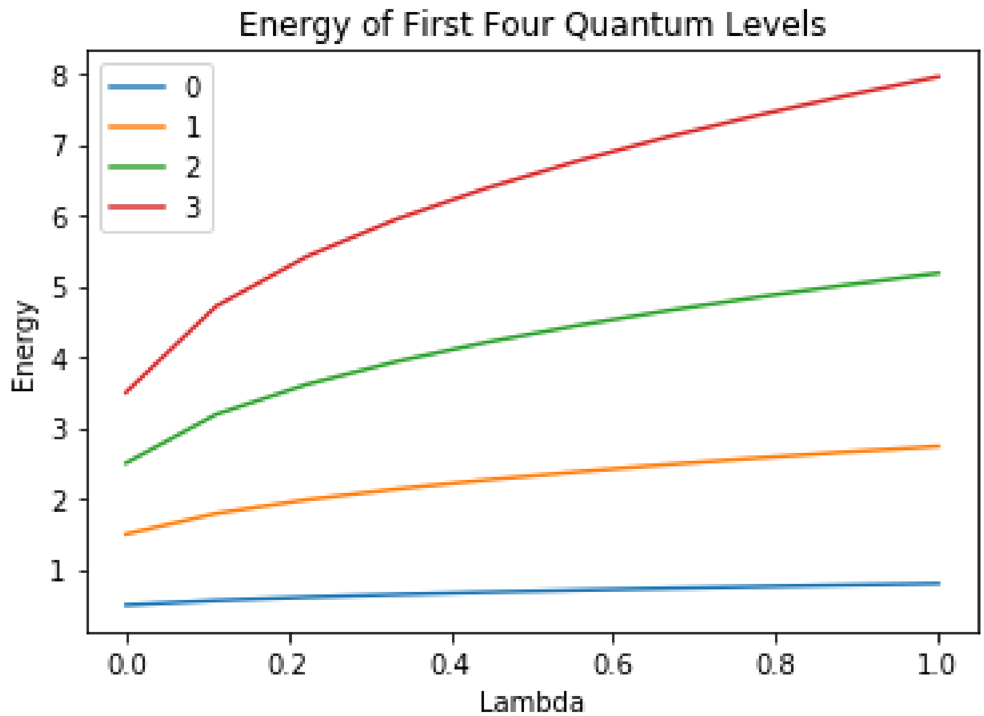
where $\hat{H}_\lambda$ is the complete hamiltonian, $\hat{H}_0$ is the hamiltonian for the harmonic oscillator, and λ is the anharmonic coefficient.

```
In [14]: import matplotlib.pyplot as plt

         #Returns the coefficient of the expanded <n|x^2|m>
         def getCoeff2(n, m):
             if n == m:
                 return (n + 0.5)
             elif n == m - 2:
                 return (0.5) * ((n + 1) * (n + 2))**(0.5)
             elif n == m + 2:
                 return (0.5) * ((n -1) * n)**(0.5)
             else:
                 return 0
```

```
#Returns the coefficient of the expanded <n|x^4|m>
def getCoeff4(n, m, upperLimit):
    sum0 = 0
    for i in range(upperLimit + 1):
        sum0 += getCoeff2(n, i) * getCoeff2(i, m)
    return sum0

#Returns the eigenvalues and eigenvector matrix of the anharmonic oscillator
def solveAnharmonic(n, coeff):
    M = np.zeros((n, n), dtype = complex)
    for i in range(n):
        for k in range(n):
            if i == k:
                M[i, k] = (0.5 + k) + (coeff * (getCoeff4(i, k, n)))
            else:
                M[i , k] = (coeff * (getCoeff4(i, k, n)))

    d, U = hermitian_eigensystem(M, 0.01)
    return d, U

#Calculates the energies of the first four quantum numbers based on the lambda value
def getEnergies(lamNum, size):
    firstEnergies = np.zeros((lamNum, 4), dtype=float)
    lambdas = np.linspace(0, 1, num=lamNum)
    for l in range(lamNum):
        d, U = solveAnharmonic(size, lambdas[l])
        firstEnergies[l, :] = d[:4]
    return firstEnergies
```

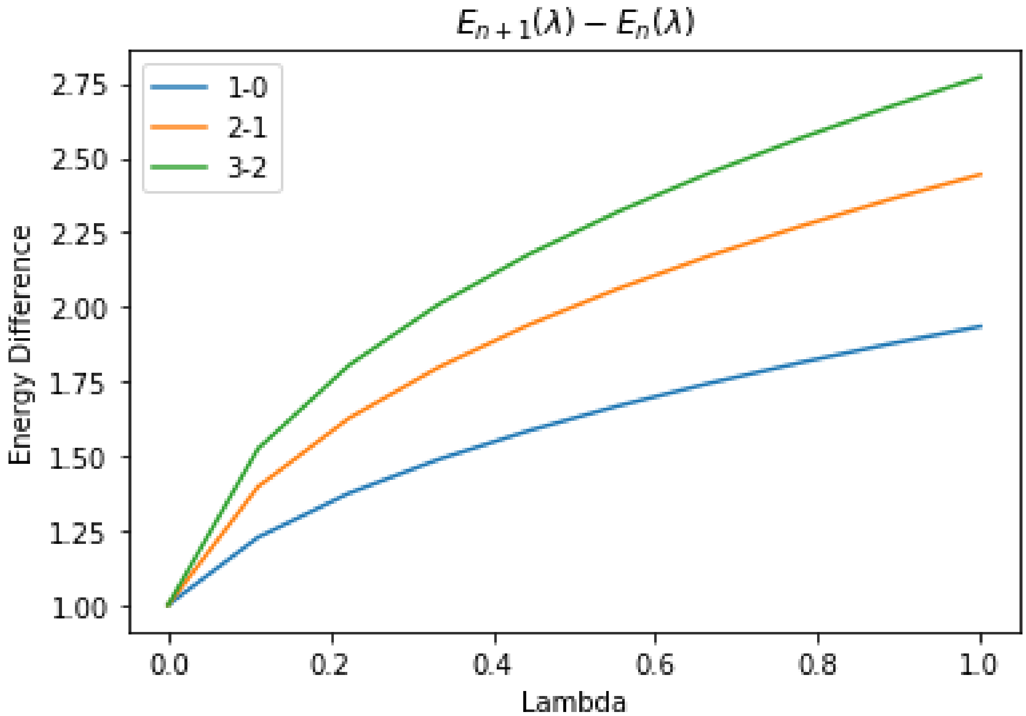
1.2.1 Energy Observations

```
In [19]: firstEnergies = getEnergies(10, 20)

         lambdas = np.linspace(0, 1, num=10)
         for i in range(4):
             plt.plot(lambdas, firstEnergies[:, i])


         plt.legend(("0", "1", "2", "3"))
         plt.xlabel("Lambda")
         plt.ylabel("Energy")
         plt.title("Energy of First Four Quantum Levels")
         plt.show()
```



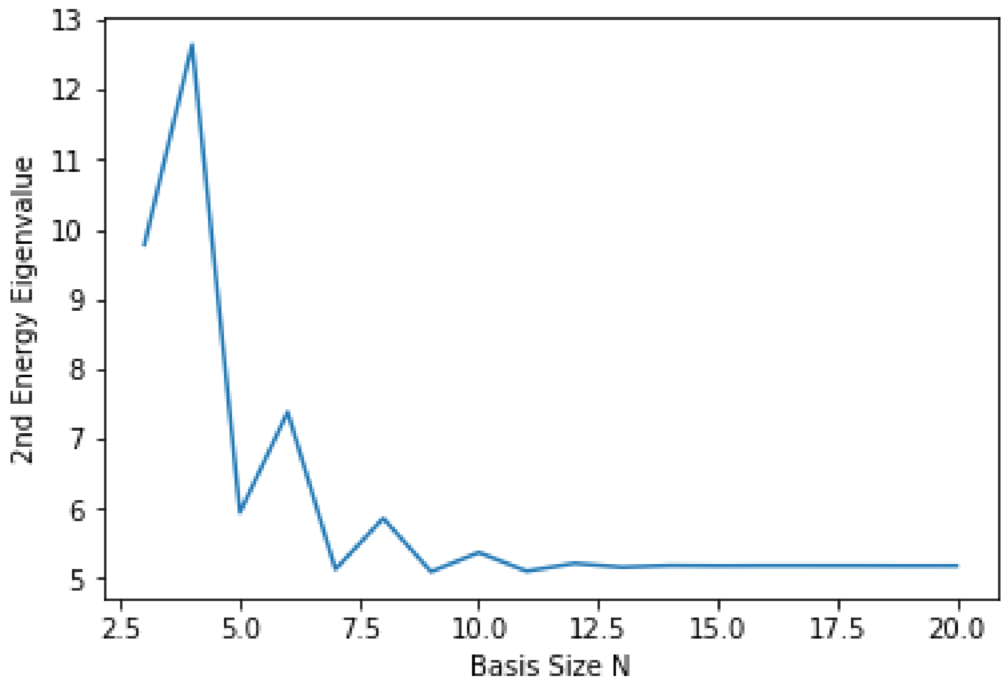
As the system becomes more anharmonic (increasing lambda value), the more energy it has for the relative quantum level. The increase in energy becomes more dramatic as the quantum level increases.

```
In [22]: differences = np.zeros((firstEnergies.shape[0], firstEnergies.shape[1] - 1), dtype = :
         for i in range(3):
             differences[:, i] = firstEnergies[:, i + 1] - firstEnergies[:, i]
             plt.plot(lambdas, differences[:, i])


         plt.legend(("1-0", "2-1", "3-2"))
         plt.xlabel("Lambda")
         plt.ylabel("Energy Difference")
         plt.title("$E_{n+1}(\lambda) - E_n(\lambda)$")
         plt.show()
```



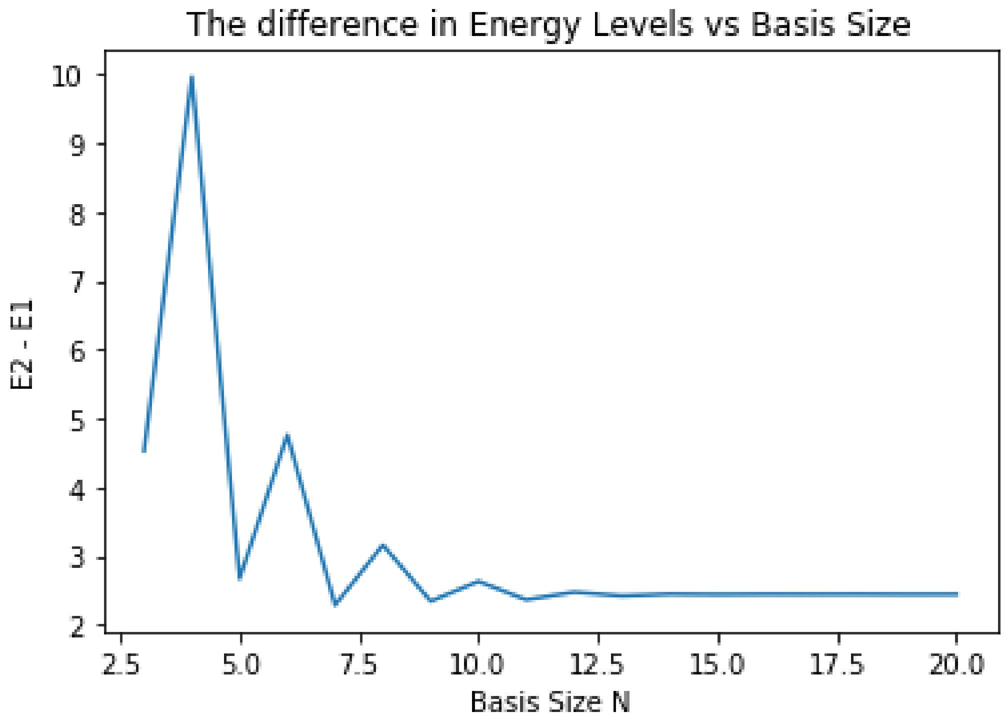
The difference in energy between adjacent quantum levels increases as (1) lambda increases and (2) as the compared quantum levels increase.

```
In [23]: def getEnergiesN(nMax, numE):
             energies = np.zeros((numE, nMax - numE), dtype = float)
             n = np.arange(numE + 1, nMax + 1)
             for i in range(len(n)):
                 d, U = solveAnharmonic(n[i], 1)
                 energies[:, i] = d[1:numE + 1]
             return energies, n

         energies, n = getEnergiesN(20, 2)

         plt.plot(n, energies[1,:])
         plt.xlabel("Basis Size N")
         plt.ylabel("2nd Energy Eigenvalue")
         plt.title("Energy vs Basis Size")
         plt.show()
```



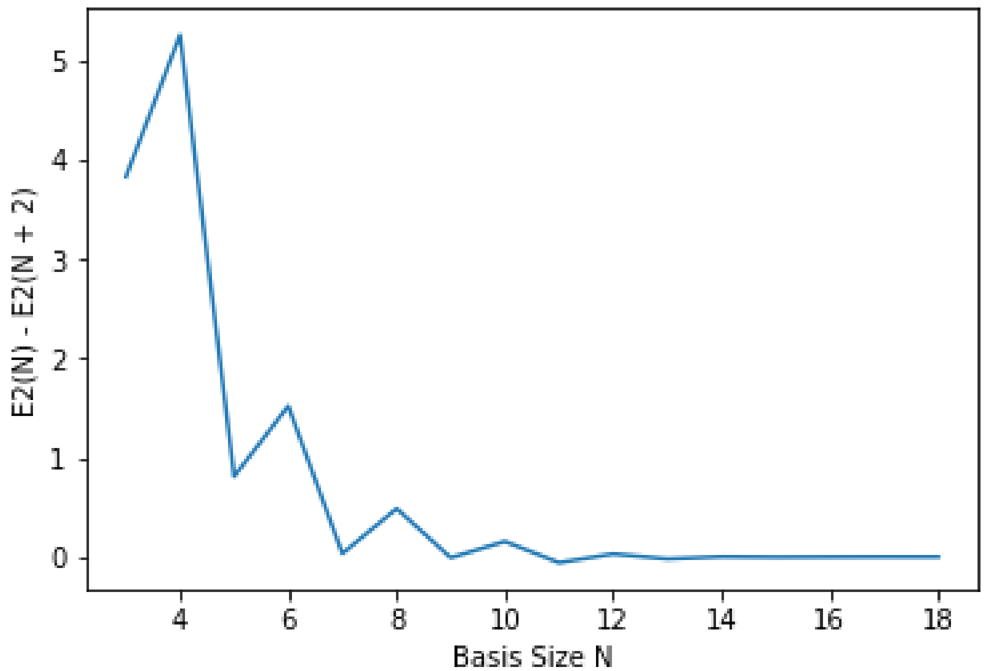
Here, it can be seen that as the basis size of the matrix increases, the 2nd energy value for the anharmonic oscillator ($\lambda = 1$) converges to around 5. The larger the basis used, the more accurate the result.

```
In [30]: differences = energies[1,:] - energies[0,:]
         plt.plot(n, differences)
         plt.xlabel("Basis Size N")
         plt.ylabel("E2 - E1")
         plt.title("The difference in Energy Levels vs Basis Size")
         plt.show()
```



The plot above illustrates how the difference between the second and first energy values converges as the basis size increases. Again, the larger basis size gives more accurate results.

```
In [25]: differences = np.array([energies[1, i] - energies[1, i + 2] for i in range(len(n) - 2

         plt.plot(n[:16], differences)
         plt.xlabel("Basis Size N")
         plt.ylabel("E2(N) - E2(N + 2)")
         plt.title("Energy Difference Between Different Basis Sizes")
         plt.show()
```

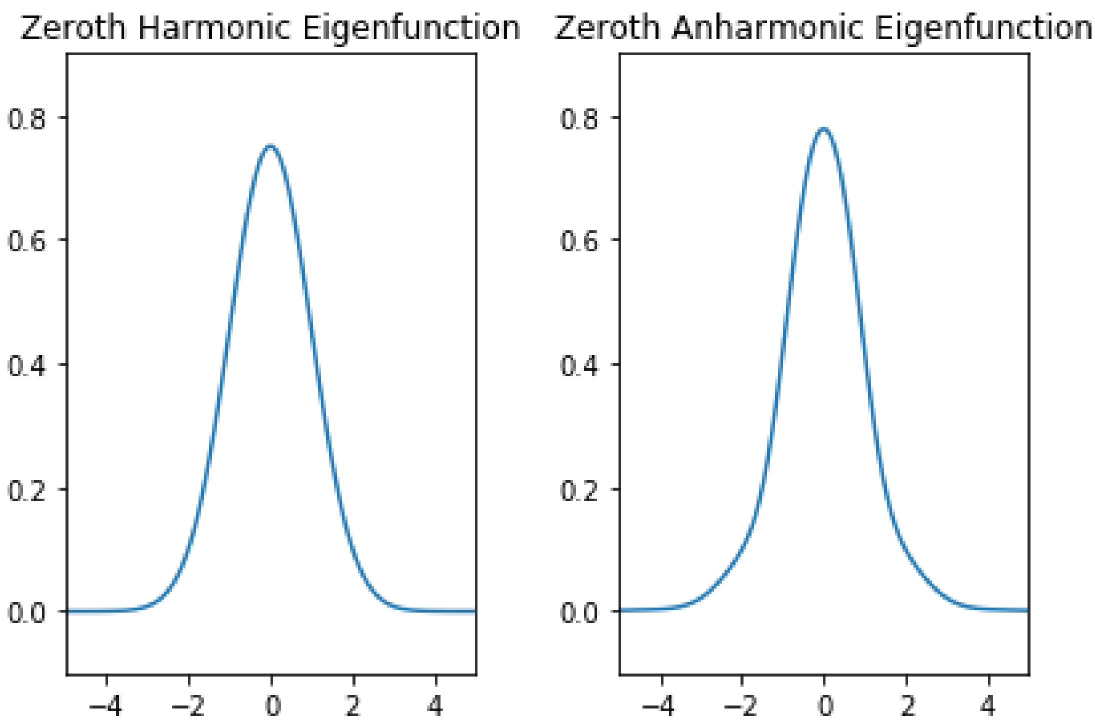


The plot above shows that difference between in the second level energy value between a basis of size N and a basis of size N+2 converges to 0. This signifies that at large N, changing the basis size won't affect the energy eigenvalue at a significant level.

1.2.2 Illustrating the Eigenfunctions

In [26]:
```
import math

#The exact solution for the harmonic oscillator
def eigenFunction(x, n, hFunc):
    coeff = ((2**n) * (math.factorial(n)) * ((np.pi)**(0.5)))**(-0.5)
    return coeff * np.exp(-(x**2)/(2)) * hFunc(x, n)

def hFunction(x, n):
    if n == 0:
        return 1
    if n == 1:
        return x * 2
    return (2 * x * hFunction(x, n - 1)) - (2 * n * hFunction(x, n - 2))



xvals = np.linspace(-5, 5, num = 100)
plt.subplot(1, 2, 1)
plt.plot(xvals, eigenFunction(xvals, 0, hFunction))
```

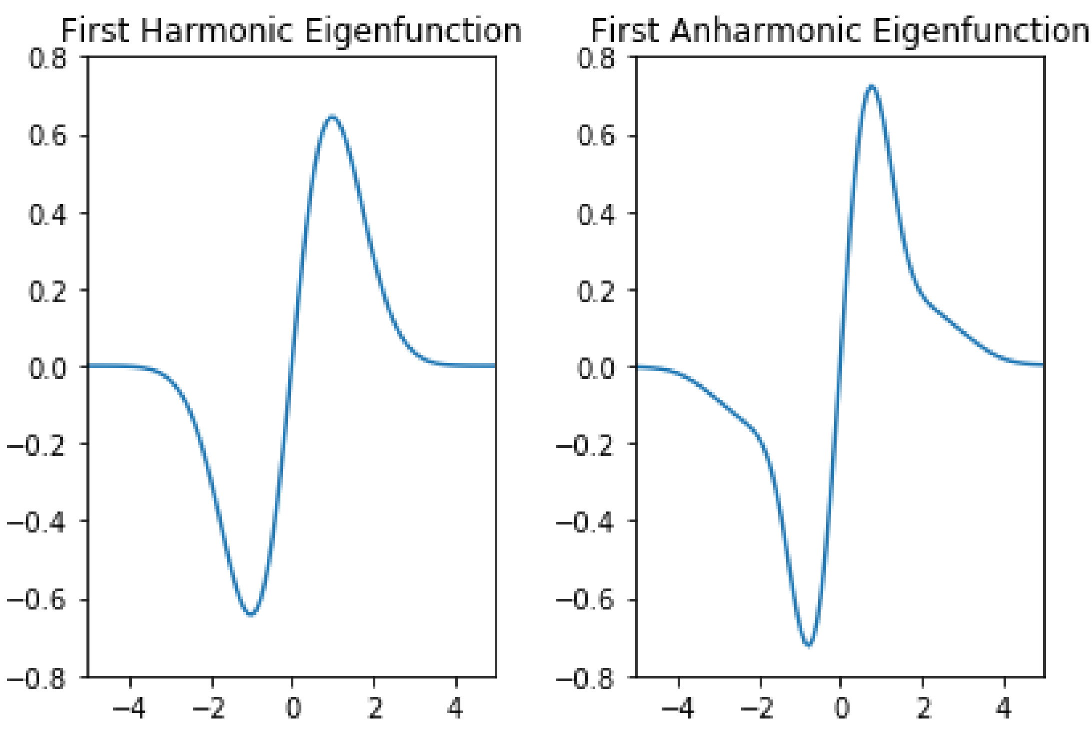
```
plt.title("Zeroth Harmonic Eigenfunction")
plt.axis([-5, 5, -.1, 0.9])

size = 20
d, U = solveAnharmonic(size, 1)
yvals = np.zeros(xvals.shape, dtype=float)
for i in range(size):
    x = 0.0
    if U[i, 0].real > U[i, 0].imag:
        x = U[i, 0].real
    else:
        x = U[i, 0].imag
    yvals += x * eigenFunction(xvals, i, hFunction)
plt.subplot(1, 2, 2)
plt.plot(xvals, yvals)
plt.title("Zeroth Anharmonic Eigenfunction")
plt.axis([-5, 5, -.1, .9])

plt.tight_layout()
plt.show()
```



It can be seen above that for the zeroth order eigenfunction, the harmonic and anharmonic eigenfunctions are very similar.

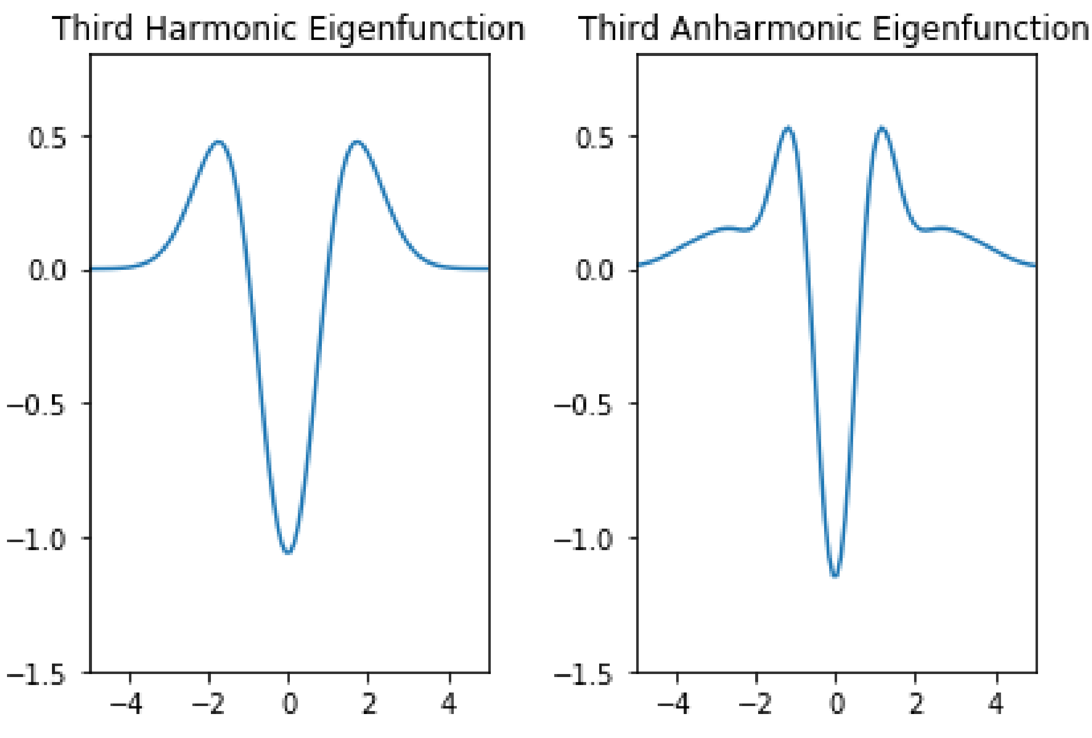
```
In [27]: plt.subplot(1, 2, 1)
```

```
plt.plot(xvals, eigenFunction(xvals, 1, hFunction))
plt.title("First Harmonic Eigenfunction")
plt.axis([-5, 5, -.8, 0.8])


yvals = np.zeros(xvals.shape, dtype=float)
for i in range(size):
    x = 0.0
    if U[i, 1].real > U[i, 1].imag:
        x = U[i, 1].real
    else:
        x = U[i, 1].imag
    yvals += x * eigenFunction(xvals, i, hFunction)

plt.subplot(1, 2, 2)
plt.plot(xvals, yvals)
plt.title("First Anharmonic Eigenfunction")
plt.axis([-5, 5, -.8, 0.8])

plt.tight_layout()
plt.show()
```



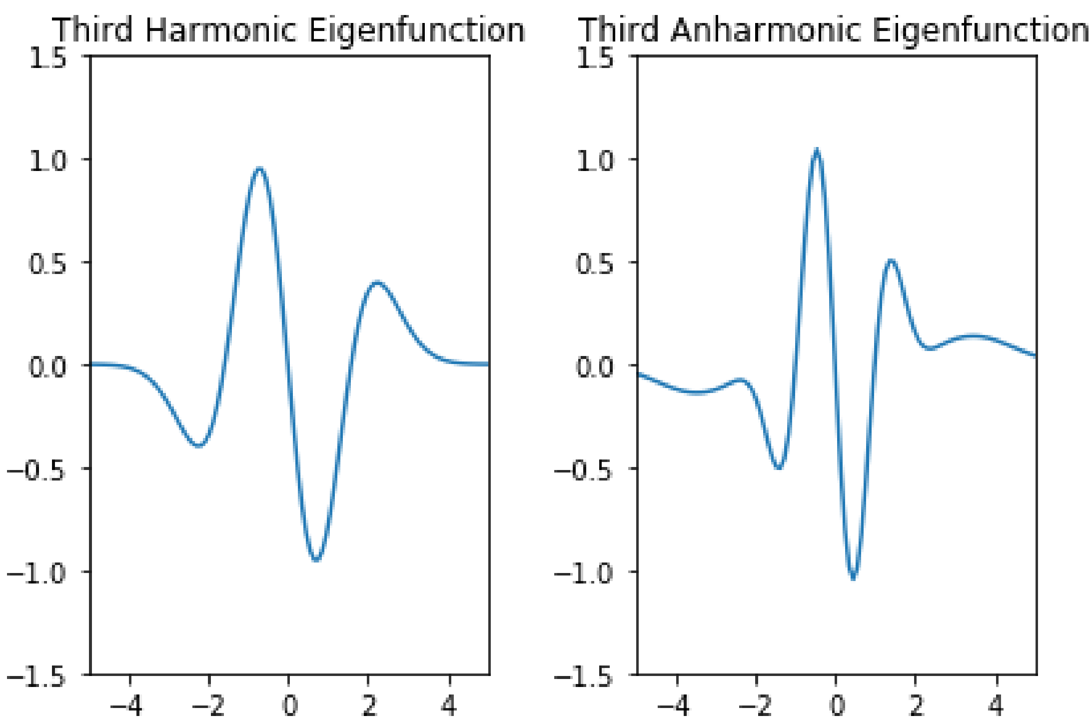

```
In [28]: plt.subplot(1, 2, 1)
         plt.plot(xvals, eigenFunction(xvals, 2, hFunction))
```

```
plt.title("Third Harmonic Eigenfunction")
plt.axis([-5, 5, -1.5, 0.8])

yvals = np.zeros(xvals.shape, dtype=float)
for i in range(size):
    x = 0.0
    if U[i, 2].real > U[i, 2].imag:
        x = U[i, 2].real
    else:
        x = U[i, 2].imag
    yvals += x * eigenFunction(xvals, i, hFunction)
plt.subplot(1, 2, 2)
plt.plot(xvals, yvals)
plt.title("Third Anharmonic Eigenfunction")
plt.axis([-5, 5, -1.5, 0.8])

plt.tight_layout()
plt.show()
```




```
In [29]: plt.subplot(1, 2, 1)
         plt.plot(xvals, eigenFunction(xvals, 3, hFunction))
         plt.title("Third Harmonic Eigenfunction")
         plt.axis([-5, 5, -1.5, 1.5])
```

```python
yvals = np.zeros(xvals.shape, dtype=float)
for i in range(size):
    x = 0.0
    if U[i, 3].real > U[i, 3].imag:
        x = U[i, 3].real
    else:
        x = U[i, 3].imag
    yvals += x * eigenFunction(xvals, i, hFunction)
plt.subplot(1, 2, 2)
plt.plot(xvals, yvals)
plt.title("Third Anharmonic Eigenfunction")
plt.axis([-5, 5, -1.5, 1.5])

plt.tight_layout()
plt.show()
```



As the order of the eigenfunction increases, the differences between the harmonic solution and the anharmonic solution become more noticeable.