**QUESTIONS PART 2:**

1) The calculated the ground state energy for the ordinary particle in a box system (with the delta function potential) that was **0.16573541893898724**. This value is greater than ground state energy (0.049298) calculated from equation (1). Output of the run is shown below:

In [**14**]: runfile('/Users/melissasuchanek/Desktop/Linear Variaional Method-Homework-2/Energy-Ground State Energy for 3\*3 basis functions1.py', wdir='/Users/melissasuchanek/Desktop/Linear Variaional Method-Homework-2')

[[ 2.49348022e-01 2.44929360e-17 -2.00000000e-01]

[ 2.44929360e-17 1.97392088e-01 -2.44929360e-17]

[-2.00000000e-01 -2.44929360e-17 6.44132198e-01]]

**0.6441321980490211- Trial Energy**

**0.16573541893898724-Ground State Energy**

[-9.22618887e-01 3.85712834e-01 6.61272129e-16]

The ground state energy without the delta function potential is 0.04934802200544679. Output of the run is shown below:

In [**2**]: runfile('/Users/melissasuchanek/Desktop/Figen Files/untitled1.py', wdir='/Users/melissasuchanek/Desktop/Figen Files')

[[0.04934802 0. 0. ]

[0. 0.19739209 0. ]

[0. 0. 0. ]]

0.0

**0.04934802200544679-Ground State Energy**

[1. 0. 0.]

The ground state energy for the ordinary particle in a box can be calculated with the following assumptions for our system m = 1, L = 10 and h (hbar) = 1 and n = 1 (the lowest energy level).

E1= (n2\*pi2\*h2) / (2\*m\*L2 ) = (1\*(3.14)2\*1) / (2\*1\*100) = 0.049298 (1)

So, the calculated energy for the ordinary particle in a box without the delta function potential is 0.04934802200544679, slightly greater than 0.049298, the ground state energy calculated from equation 1. The difference between the energies is 5.0022E-5.

2) In a box system with an ordinary particle, mixing in functions that correspond to excited states helped lower the energy in the system with delta function potential. The excited state is known as a quantum state with higher energy than the initial ground state.

When a pulse is applied to the system, the system is disturbed. For example, in our particle in a box system, the box was deformed by applying the potential energy with a delta function. As a result, all the excited energy levels are disturbed and they are losing energy, which in turn lowers the ground state energy.

3) When the number of basis functions is increased to 6 (which is a 6x6 matrix and is a vector with 6 entries), the estimate of the ground state energy is expected to be lower compared to when there are 3 (which is a 3x3 matrix and is a vector with 3 entries) basis functions (more eigen vectors cover more space to reach to the limit in addition expansion of coefficients vectors, both of which lower the ground state energy)

Some of the coefficients for 6\*6 matrix-basis functions are smaller than the coefficients 3\*3 matrix-basis functions 3 (3.8571e-01 >-9.34136379e-01 Please see Table 1.

**The energy for 6\*6 matrix-basis functions 6**

In [**15**]: runfile('/Users/melissasuchanek/Desktop/Linear Variaional Method-Homework-2/Energy-Ground State Energy for 6\*6 basis functions1.py', wdir='/Users/melissasuchanek/Desktop/Linear Variaional Method-Homework-2')

[[ 2.49348022e-01 2.44929360e-17 -2.00000000e-01 -4.89858720e-17

2.00000000e-01 7.34788079e-17]

[ 2.44929360e-17 1.97392088e-01 -2.44929360e-17 -5.99903913e-33

2.44929360e-17 8.99855870e-33]

[-2.00000000e-01 -2.44929360e-17 6.44132198e-01 4.89858720e-17

-2.00000000e-01 -7.34788079e-17]

[-4.89858720e-17 -5.99903913e-33 4.89858720e-17 7.89568352e-01

-4.89858720e-17 -1.79971174e-32]

[ 2.00000000e-01 2.44929360e-17 -2.00000000e-01 -4.89858720e-17

1.43370055e+00 7.34788079e-17]

[ 7.34788079e-17 8.99855870e-33 -7.34788079e-17 -1.79971174e-32

7.34788079e-17 1.77652879e+00]]

**2.4206609902451057- Trial Energy**

**1.527752265195961-Ground State**

[-1.88514391e-01 -9.34136379e-01 3.03070206e-01 -1.16345328e-16

4.97468397e-16 1.10085006e-16]

**The energy for 3\*3 matrix-basis functions 3**

In [**14**]: runfile('/Users/melissasuchanek/Desktop/Linear Variaional Method-Homework-2/Energy-Ground State Energy for 3\*3 basis functions1.py', wdir='/Users/melissasuchanek/Desktop/Linear Variaional Method-Homework-2')

[[ 2.49348022e-01 2.44929360e-17 -2.00000000e-01]

[ 2.44929360e-17 1.97392088e-01 -2.44929360e-17]

[-2.00000000e-01 -2.44929360e-17 6.44132198e-01]]

**0.6441321980490211- Trial Energy**

**0.16573541893898724-Ground State**

[-9.22618887e-01 3.85712834e-01 6.61272129e-16]

Table 1. The coefficient relations between 3\*3 and 6\*6 matrices.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Coefficients | Coefficients | Coefficients | Coefficients | Coefficients | Coefficients |
| 3\*3 Matrix | -9.2267e-01 | 3.8571e-01 | 6.6127e-16 |  |  |  |
| 6\*6 Matrix | -1.8851e-01 | -9.3413e-01 | 3.0307e-01 | -1.16348e-16 | 4.9746e-16 | 1.10085e-16 |