Solution #8

Question A: ANHARMONIC OSCILLATOR

The goal of this problem is to find numerically the low lying spectrum of an anharmonic oscillator:

$$H = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 + \lambda\hat{x}^4. \tag{1}$$

We will do this numerically following these steps:

1. Choose a basis of the Hilbert space. I strongly suggest you choose the basis of eigenstates of the harmonic oscillator (without the anharmonic part).
2. Calculate the matrix representation of H in this basis. This is an infinite matrix so you can only calculate a finite number of terms, say, a 10×10 matrix. This can and should be done analytically. You can use a computer or, even better, compute a few terms as guess the pattern. Using the harmonic oscillators raising and lowering operators helps a lot.
3. Pick the values of the parameters: $\hbar = \omega = 1$. For different values of λ find the eigenvalues of the matrix $\langle |an|\hat{H}|m\rangle$.
4. Make a plot of the ground state energy as a function of λ and compared it with the results given by perturbation theory you worked out last week.
5. Do you think the 10 energy levels you kept are enough to give a 1% precision in the ground state energy? If not, how many you should keep?
6. One may wonder how hard it would be to use this method for some more interesting problem like, say, the ground state of the oxygen atom. We could use as a basis the eigenstates of the hamiltonian including the kinetic energy of the electrons and the Coulomb interaction between electrons and the nucleus (but not the Coulomb repulsion between the the electrons). The wave function are known analytically so one should be able to compute the matrix elements needed. Suppose we include all the states up (and including) the $n = 5$ states. How large would be the matrix to be numerical diagonalised? (As large as this may be, the main problem would be the computation of the matrix elects as each one would be a 6-dimensional integral. Can you see why?)

Answer:

1. We choose the basis of eigenstates of the standard harmonic oscillator.
2. Using raising and lowering operators, $\hat{H}_0 = \hbar\omega(a_+a_- + \frac{1}{2})$.

Since $a_+a_- |n\rangle = N |n\rangle, \langle m| H_0 |n\rangle = \hbar\omega(N + \frac{1}{2}) \langle m| |n\rangle$

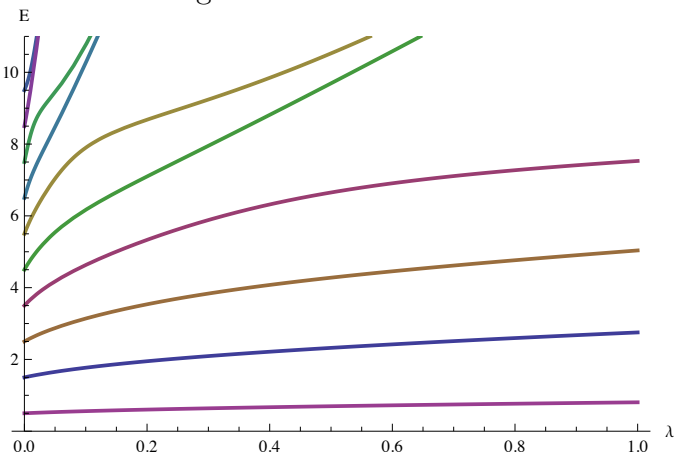
For $\hat{H}' = \lambda\hat{x}^4, \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-) = (a_+ + a_-)$, we get the matrix of x,

$$\begin{pmatrix}
0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{\sqrt{2}} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \sqrt{\frac{3}{2}} & 0 & \sqrt{2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \sqrt{2} & 0 & \sqrt{\frac{5}{2}} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \sqrt{\frac{5}{2}} & 0 & \sqrt{3} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \sqrt{3} & 0 & \sqrt{\frac{7}{2}} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \sqrt{\frac{7}{2}} & 0 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & \frac{3}{\sqrt{2}} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{\sqrt{2}} & 0
\end{pmatrix}$$

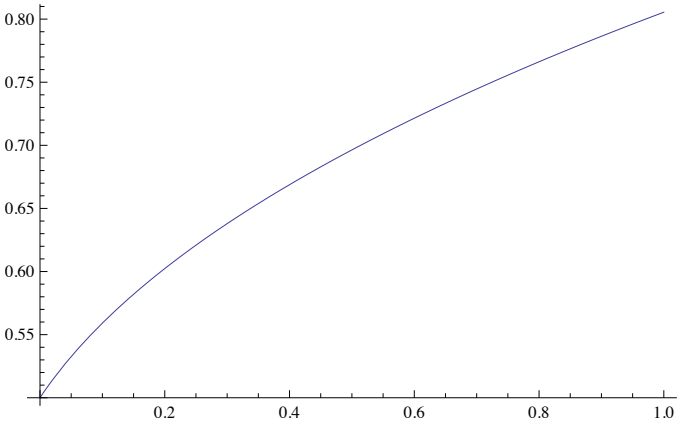
Since $H = H_0 + \lambda x^4$, we use the matrix products, and get the whole presentation of H:

$$\begin{pmatrix}
\frac{1}{2}+\frac{3\lambda}{4} & 0 & \frac{3\lambda}{\sqrt{2}} & 0 & \sqrt{\frac{3}{2}}\,\lambda & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{3}{2}+\frac{15\lambda}{4} & 0 & \left(3\sqrt{\frac{3}{2}}+\sqrt{6}\right)\lambda & 0 & \sqrt{\frac{15}{2}}\,\lambda & 0 & 0 & 0 & 0 \\
\frac{3\lambda}{\sqrt{2}} & 0 & \frac{5}{2}+\left(3+\sqrt{\frac{3}{2}}\left(\frac{5\sqrt{\frac{5}{2}}}{2}+\sqrt{6}\right)\right)\lambda & 0 & \left(\frac{5\sqrt{3}}{2}+\sqrt{2}\left(\frac{5\sqrt{\frac{5}{2}}}{2}+\sqrt{6}\right)\right)\lambda & 0 & 3\sqrt{\frac{5}{2}}\,\lambda & 0 & 0 & 0 \\
0 & 5\sqrt{\frac{3}{2}}\,\lambda & 0 & \frac{7}{2}+\frac{75\lambda}{4} & 0 & 9\sqrt{5}\,\lambda & 0 & \sqrt{\frac{105}{2}}\,\lambda & 0 & 0 \\
\sqrt{\frac{3}{2}}\,\lambda & 0 & 7\sqrt{3}\,\lambda & 0 & \frac{9}{2}+\frac{123\lambda}{4} & 0 & 11\sqrt{\frac{15}{2}}\,\lambda & 0 & \sqrt{105}\,\lambda & 0 \\
0 & \sqrt{\frac{15}{2}}\,\lambda & 0 & \left(\frac{3\sqrt{5}}{2}+\sqrt{2}\left(\frac{11\sqrt{\frac{5}{2}}}{2}+\sqrt{10}\right)\right)\lambda & 0 & \frac{11}{2}+\left(27+\sqrt{\frac{5}{2}}\left(\frac{11\sqrt{\frac{5}{2}}}{2}+\sqrt{10}\right)\right)\lambda & 0 & \left(9\sqrt{\frac{21}{2}}+2\sqrt{42}\right)\lambda & 0 & 3\sqrt{21}\,\lambda \\
0 & 0 & 3\sqrt{\frac{5}{2}}\,\lambda & 0 & \left(9\sqrt{\frac{15}{2}}+\sqrt{30}\right)\lambda & 0 & \frac{13}{2}+\left(27+\sqrt{\frac{7}{2}}\left(\frac{13\sqrt{\frac{7}{2}}}{2}+2\sqrt{14}\right)\right)\lambda & 0 & \left(9\sqrt{\frac{7}{2}}+2\left(\frac{13\sqrt{\frac{7}{2}}}{2}+2\sqrt{14}\right)\right)\lambda & 0 \\
0 & 0 & 0 & \sqrt{\frac{105}{2}}\,\lambda & 0 & 13\sqrt{\frac{21}{2}}\,\lambda & 0 & \frac{15}{2}+\frac{339\lambda}{4} & 0 & 36\sqrt{2}\,\lambda \\
0 & 0 & 0 & 0 & \sqrt{105}\,\lambda & 0 & 15\sqrt{14}\,\lambda & 0 & \frac{17}{2}+\frac{345\lambda}{4} & 0 \\
0 & 0 & 0 & 0 & 0 & 3\sqrt{21}\,\lambda & 0 & \left(\frac{21}{\sqrt{2}}+2\left(\frac{27}{2\sqrt{2}}+6\sqrt{2}\right)\right)\lambda & 0 & \frac{19}{2}+\frac{3\left(\frac{27}{2\sqrt{2}}+6\sqrt{2}\right)\lambda}{\sqrt{2}}
\end{pmatrix}$$

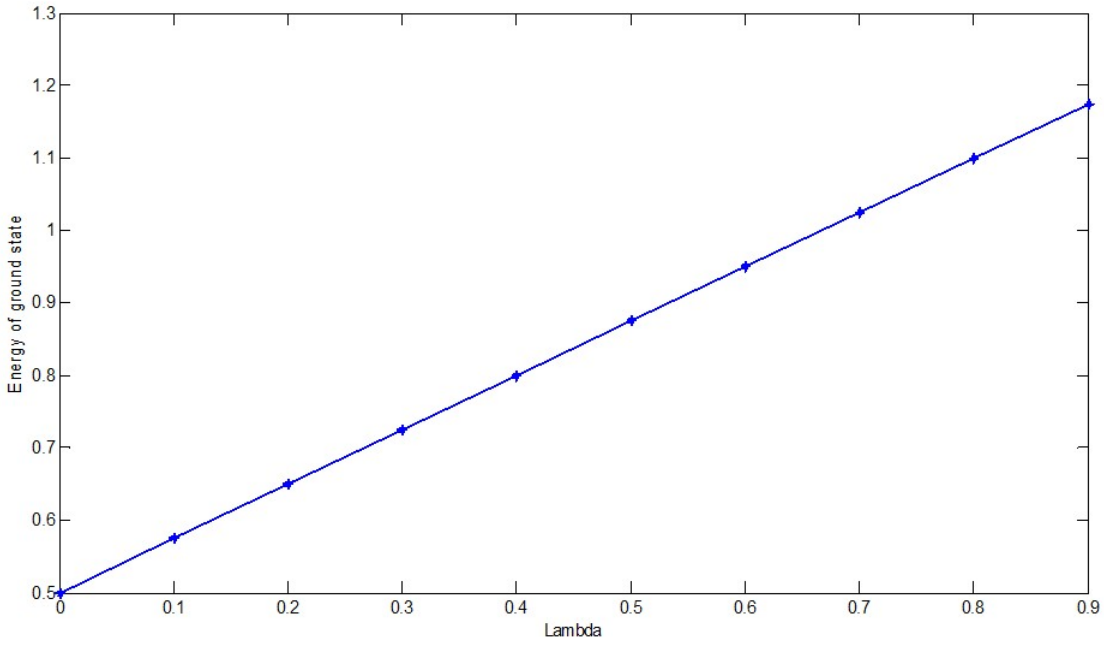
3. We assume $m = \hbar = \omega = 1$ to solve the eigenvalue of above matrices. Choosing λ from 0 to 0.9 by step of 0.1, we get ten sets of data, shown in the below plot. For every λ, we have ten eigenvalues.

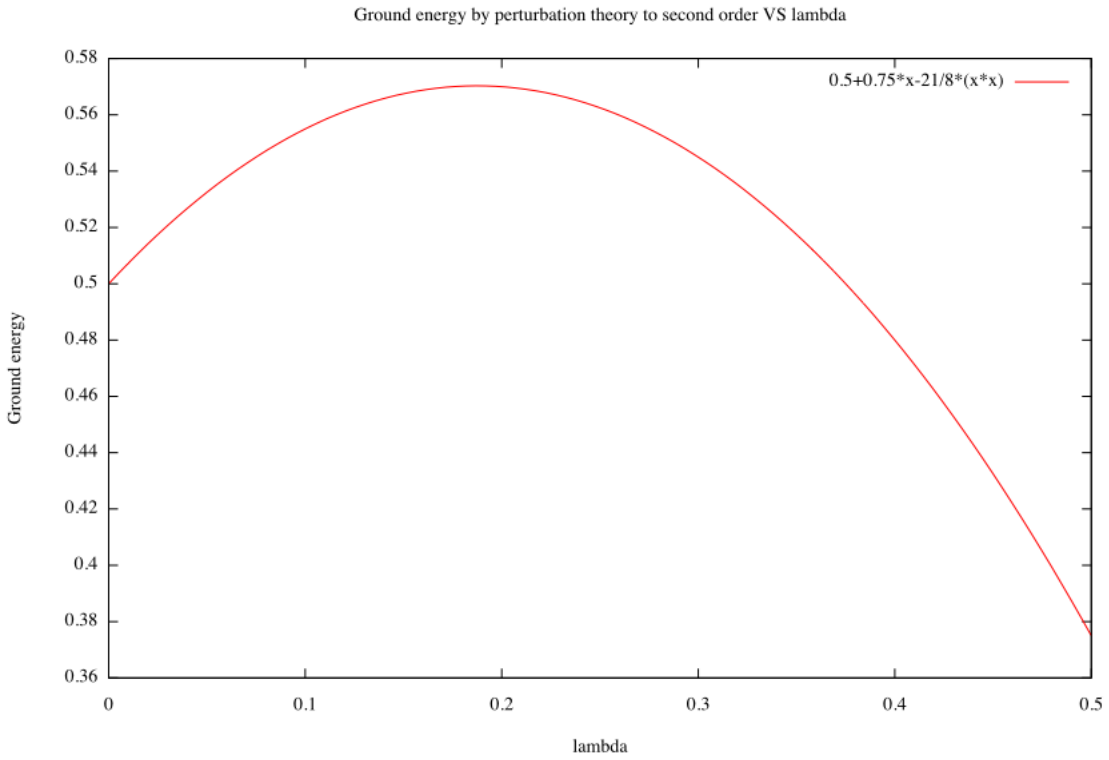


4. The ground state energy for every level is given in below plot. Actually it is the zoom in of purple line in above plot.



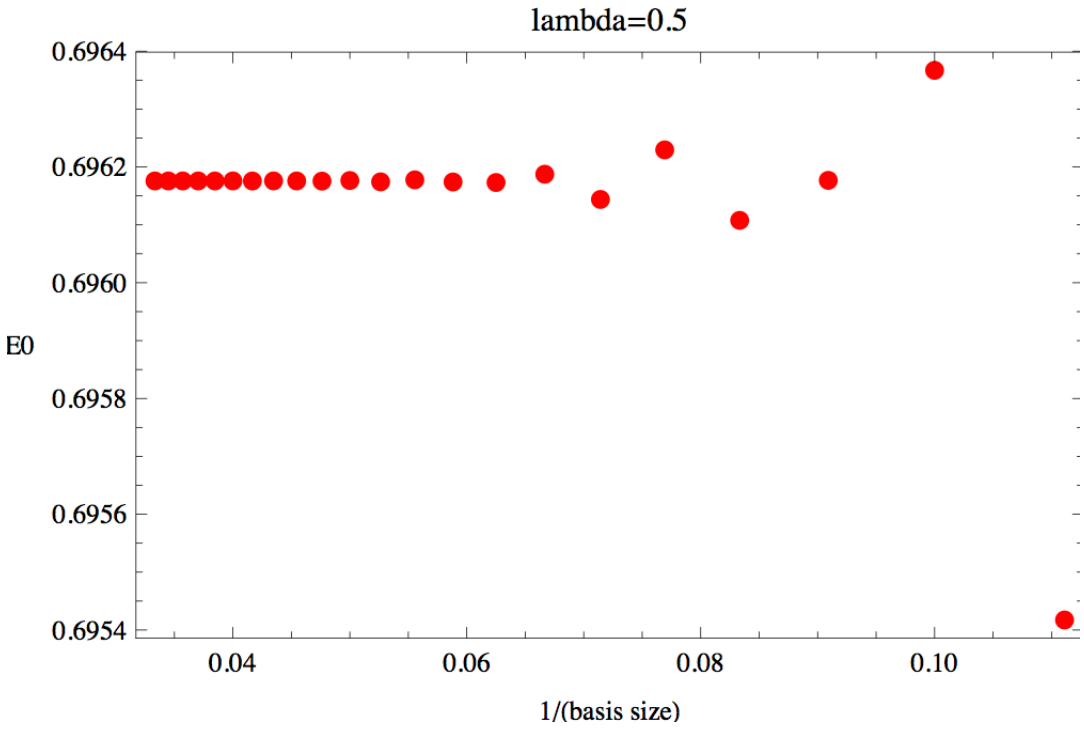
Recall what did about the perturbation theory in last homework, and using the assumption $m = \hbar = \omega = 1$,we have $H_{groundstate} = \frac{1}{2} + \frac{3}{4}\lambda - \frac{21}{8}\lambda^2$. The second and third terms are the first and second order correction respectively. The next two plots are plots of first and second corrections respectively.

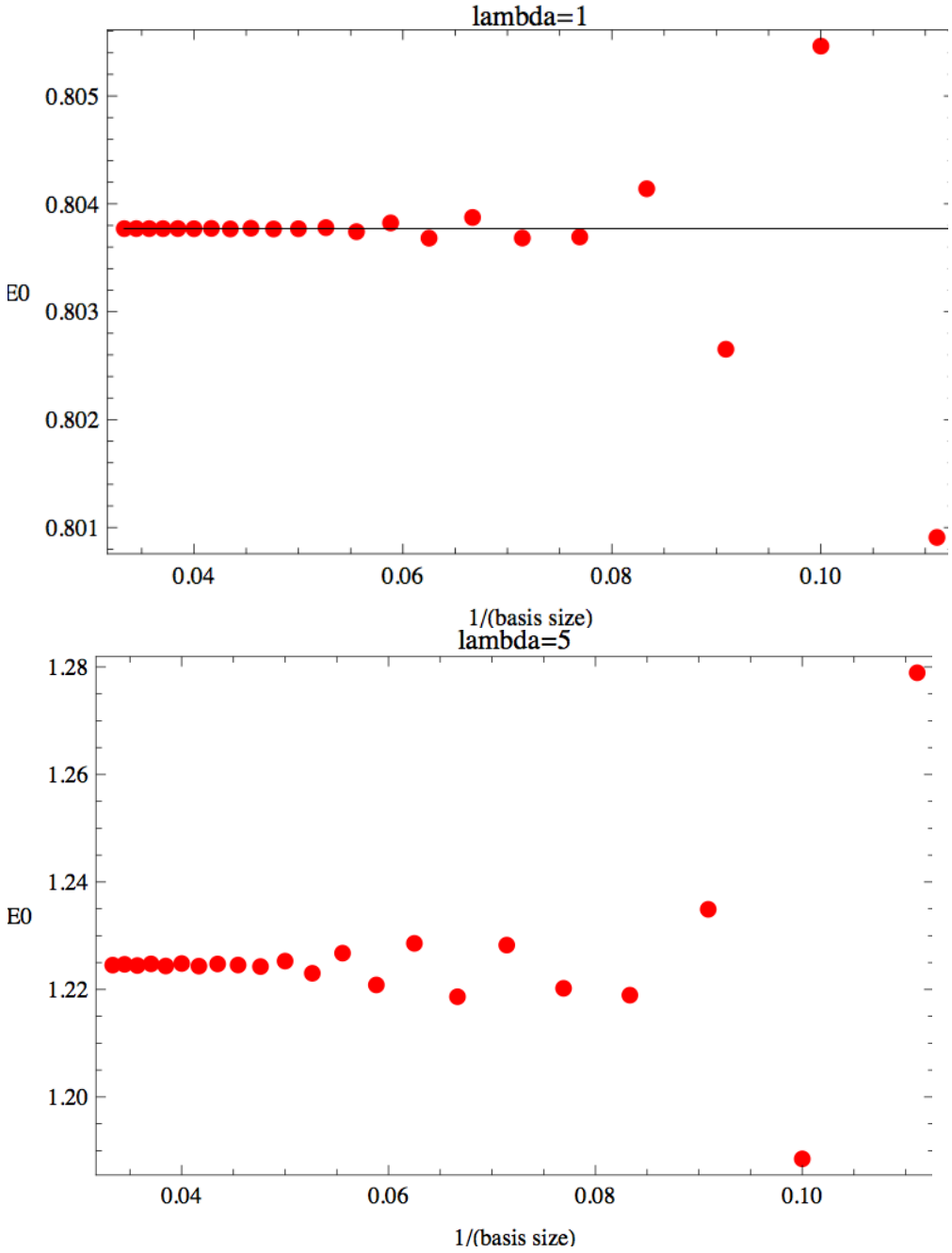




We noticed that within $\lambda = 0.1$, both second and first order perturbation work fine.

5. It is easy to guess that with $\lambda increasing$, more energy levels(bigger matrix) are needed to estimate the energy. We hope to get converged energy within those ten basis H matrix. Here I plot three cases, for $\lambda = 0.5, 1, 5$





From those examples, we clearly see for λ smaller than 1, basis =10 are enough to get 0.1% precision. Even until $\lambda = 5$, the precision becomes more than 1% and bigger scale matrix are needed to get more exact values.

Question B: Non-degenerate Pertubation theory

A quantum system has a three-dimensional Hilbert space and a hamiltonian whose matrix in a creation orthonormal basis is

$$H = \underbrace{E_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{H_0} + \underbrace{\lambda \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{V}. \tag{2}$$

1. Find the eigenvalues of H exactly.
2. We will pretend to forget the previous item and attempt to use perturbation theory to find the eigenvalues of H. The problem is that H_0 is degenerate. One should use non-degenerate perturbation theory to compute the spectrum correction due to V but let us pretend we don't know that, use the H_0 eigenbasis

$$\psi_a = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \psi_b = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \psi_c = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \tag{3}$$

   and compute the shift in the energy eigenvalues using first order perturbation theory. How does that compare with the exact answer?

3. What happens if you try to compute the shift in the eigenstates using first order perturbation theory using the $\psi_{Aa,b,c}$ basis?
4. Use now the H_0 eigenbasis

$$\psi_A = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \psi_B = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \psi_C = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \tag{4}$$

   and compute the shift in the energy eigenvalues using first order perturbation theory. How does that compare with the exact answer?

5. Compute the new eigenstates using first order perturbation theory using the $\psi_{A,B,C}$ basis.

Answer:

1. $\hat{H} = \begin{pmatrix} E_0 & \lambda & 0 \\ \lambda & E_0 & 0 \\ 0 & 0 & E_0 \end{pmatrix}$

To get the eigenvalues α, we need $det(H - \alpha I) = 0$

$$\begin{pmatrix} E_0 - \alpha & \lambda & 0 \\ \lambda & E_0 - \alpha & 0 \\ 0 & 0 & E_0 - \alpha \end{pmatrix} = 0$$

$\implies \alpha = E_0, E_0 + \lambda, and E_0 - \lambda$

2. As we know, the first order correction to energy is $E'_n = \langle \psi_n^0 | H' | \psi_n^0 \rangle$. So:

in case of ψ_a, we have $E_a = \langle \psi_a | V | \psi_a \rangle = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & \lambda & 0 \\ \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

$\implies E_a = 0$

in case of ψ_b, we have $E_b = \langle \psi_b | V | \psi_b \rangle = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \lambda & 0 \\ \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

$\implies E_b = 0$

in case of ψ_c, we have $E_c = \langle \psi_c | V | \psi_c \rangle = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & \lambda & 0 \\ \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$\implies E_c = 0$

3. $\psi_{abc} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. It is diagonal matrix.

When using the ψ_{abc}basis, we have $E_{abc} = \langle \psi_{abc} | V | \psi_{abc} \rangle = V = \begin{pmatrix} 0 & \lambda & 0 \\ \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

We solve the eigenvalues, and get the exact correction $0, \lambda, -\lambda$

4. Now we use the eigenbasis of $\hat{H}_0$, $\psi_A = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \psi_B = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \psi_C = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

In case of ψ_A, we have $E_A = \langle \psi_A | V | \psi_A \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \lambda & 0 \\ \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$

$\Longrightarrow E_A = \lambda$

In case of ψ_B, we have $E_B = \langle \psi_B | V | \psi_B \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \lambda & 0 \\ \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$

$\Longrightarrow E_B = -\lambda$

In case of ψ_C, we have $E_C = \langle \psi_C | V | \psi_C \rangle = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & \lambda & 0 \\ \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$\Longrightarrow E_C = 0$

5. $\psi_{ABC} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$.

When using the ψ_{abc}basis, we have

$E_{ABC} = \langle \psi_{ABC} | V | \psi_{ABC} \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & \lambda & 0 \\ \lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \lambda & 0 & 0 \\ 0 & -\lambda & 0 \\ 0 & 0 & 0 \end{pmatrix}$

We solve the eigenvalues, and get the exact correction $0, \lambda, -\lambda$