QUANTUM MECHANICS II

PROBLEM SET 8

due October 31th, before class

I. 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?)

II. SIMPLE EXAMPLE OF DEGENERATE PERTURBATION 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.