Solution #9

Question A: Variational Calculation for the Anharmonic Oscilator

Use the variational ansatz

$$\psi_\alpha(x) \sim e^{-\alpha x^2} \tag{1}$$

to estimate the ground state energy of the enharmonic oscillator described by the hamiltonian

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

Notice that I'm setting $|omega = 0$ to simplify the problem. Try to repeat the "exact" calculation of the last week for the present case with $\omega = 0$ and compare it with the variational result you just got.

Answer:

$\psi_\alpha \approx e^{-\alpha x^2}$; $\hat{H} = \frac{\hat{p}^2}{2m} + \lambda \hat{x}^4$

Doing simple integral, we get A=$(\frac{2\alpha}{\pi})^{\frac{1}{4}}$

First we need to make the ansatz normalized:$\langle\psi_\alpha|\,|\psi_\alpha\rangle = 1$

The expectation value of $\hat{H}$ is: $< H_\alpha >= \langle\psi_\alpha|\,\hat{H}\,|\psi_\alpha\rangle = \int dx \psi_\alpha^*(\frac{\hat{p}^2}{2m} + \lambda\hat{x}^4)\psi_\alpha$

Given $\psi_\alpha = (\frac{2\alpha}{\pi})^{\frac{1}{4}} e^{-\alpha x^2}, \hat{p} = i\hbar\frac{d}{dx}$, we get $< H_\alpha >= \frac{\alpha\hbar^2}{2m} + \frac{3\lambda}{16\alpha^2}$

Then we minimize the expectation value, $\frac{d<H_\alpha>}{d\alpha} = 0$

$\Longrightarrow \alpha_{min} = (\frac{3m\lambda}{4\hbar^2})^{\frac{1}{3}}$

Substitute back into $< H_\alpha >$, we get $H_{min} = \frac{3\hbar^2}{4m}(\frac{3m\lambda}{4\hbar^2})^{\frac{1}{3}}$

Next some results from Mathematica are attached to compare our numerically "exact" result with this variational result.

Construct the matrices of a, a†, p and x in the unperturbed basis

```
Λ = 30;
Clear[m, λ, ω, h]
MatrixForm[ad = Table[If[j + 1 == i, Sqrt[i - 1], 0], {i, 1, Λ}, {j, 1, Λ}]];
MatrixForm[a = Transpose[ad]];
MatrixForm[p = -I Sqrt[m (h ω)/2] (a - ad)];
MatrixForm[x = Sqrt[h/(2 m ω)] (a + ad)];
```

Verify commutation relation

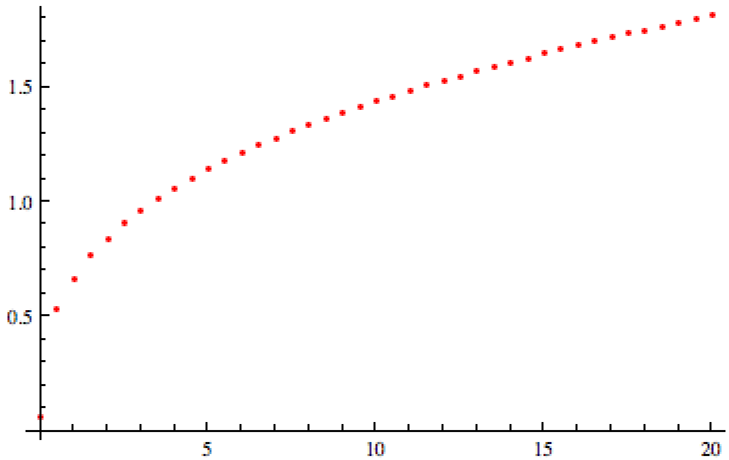
```
MatrixForm[a.ad - ad.a];
```

Verify that the harmonic oscillator hamiltonian is right

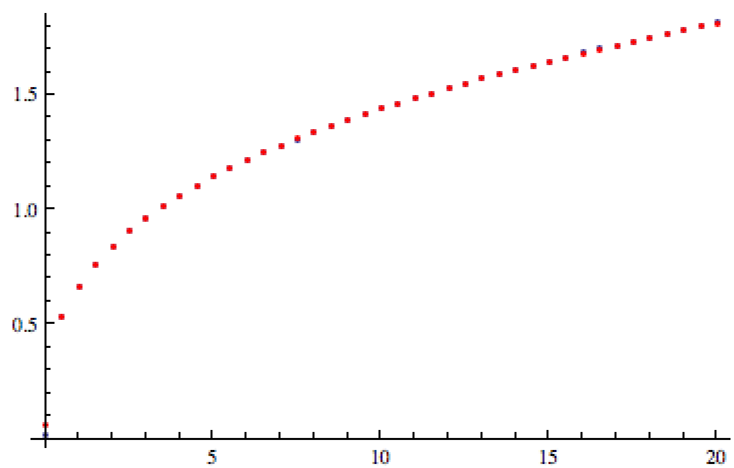
```
MatrixForm[p.p/(2 m) + m ω^2/2 x.x];
```

Compute the lowest eigenvalue for the anharmonic oscillator (in the basis of the harmonic oscillator with frequency ω which I take to be ω=3 since the energy should not depend on it for large enough Λ)

```
m = h = 1; ω = 3;
p30ω3 = ListPlot[{
    Table[{λ, Eigenvalues[H = p.p/(2. m) + 0 m ω^2/2 x.x + λ x.x.x.x][[Λ]]}, {λ, 0, 20, 0.5}]
  }, PlotStyle → Red]
Clear[m, ω, h, λ]
```

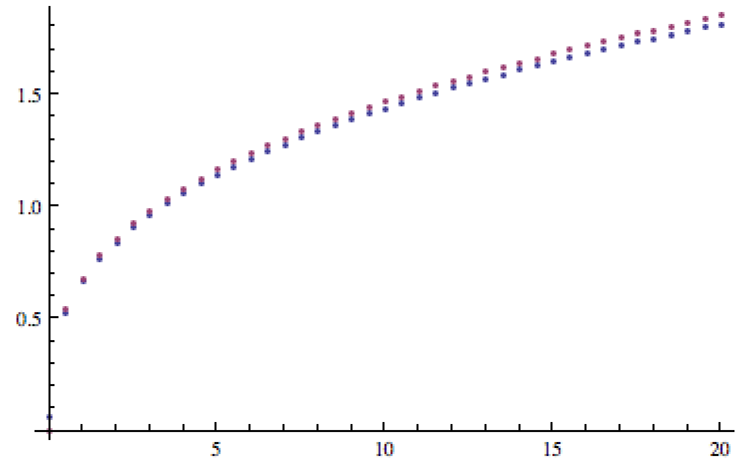



```
Show[{p30ω1, p30ω3}]
```



Compare "exact" result with variational calculation

```
m = h = 1; ω = 3;
ListPlot[{
  Table[{λ, Eigenvalues[H = p.p/(2 m) + 0 m ω^2/2 x.x + λ x.x.x.x][[Λ]]}, {λ, 0, 20, 0.5}],
  (*Table[{λ, (1/2 + λ( x.x.x.x)[[1,1]])}, {λ,0,1,0.03}],*)
  Table[{λ, Evariational}, {λ, 0, 20, 0.5}]
 }]
Clear[m, ω, h, λ]
```



Question B: Variational Method fro Excited States

Prove the following generalization of the variational principle: the first excited state is the normalized state *orthogonal to the ground state* with the smallest value of (the expectation value of) the energy. Use this result to estimate the first excited state of the harmonic oscillator. It is up to you to make a good ansatz so different people will have different solutions to this problem. How does your estimate compared to the exact solution?

Answer:

First let's write ψ in the terms of energy eigenfunctions $|\psi\rangle = \sum c_n |\psi_n\rangle$, and $\sum |c_n|^2 = 1$.
The ground state $|\psi_0\rangle$, is orthogonal to ψ. We have $\langle\psi| |\psi_0\rangle = 0$
The expectation value of H, $\langle\psi| H |\psi\rangle = \sum c_m^* c_n \langle\psi| H |\psi\rangle = \sum c_m^* c_n \langle\psi| H |\psi\rangle = \sum c_m^* c_n \delta_{mn} \langle\psi| H |\psi\rangle = \sum |c_n|^2 E_n \geq E_1 = E_1$
Try the ansatz: $\psi_\alpha = Axe^{-\alpha x^2}$. From normalization, A=$2(\frac{2\alpha^3}{\pi})^{\frac{1}{4}}$.
The expectation value of the first excited state:
$< E_\alpha >= \langle\psi_\alpha| H |\psi_\alpha\rangle = A^2 \int dx x e^{-bx^2}(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x^2} + \frac{m\omega^2 x^2}{2}) x e^{-\alpha x^2} = \frac{3\hbar^2\alpha}{2m} + \frac{3m\omega^2}{8\alpha}$
According to variational method, we minimize the expectation value, $\frac{d<E_\alpha>}{d\alpha} = 0$
$\Longrightarrow \alpha_{min} = \frac{m\omega}{2\hbar}$
$\Longrightarrow E_{min} = \frac{3\hbar\omega}{2}$
In fact our ansatz is from the wave function for the first excited state so that we get such an good estimation.

Question C: Feynman-Hellmann and the Expectation Values of $1/r$ and $1/r^2$ in Hydrogen Atom

Answer: /Griffth 6.32(a)

Feynman-Hellmann theorem states $\frac{\partial E_n}{\partial\lambda} = \langle\psi_n| \frac{\partial H}{\partial\lambda} |\psi_n\rangle$
We know $E_n = \langle\psi_n| H |\psi_n\rangle$. Then $\frac{\partial E_n}{\partial\lambda} = \langle\psi_n| \frac{\partial H}{\partial\lambda} |\psi_n\rangle + \langle\frac{\partial\psi_n}{\partial\lambda}| H |\psi_n\rangle + \langle\psi_n| H |\frac{\partial\psi_n}{\partial\lambda}\rangle = \langle\psi_n| \frac{\partial H}{\partial\lambda} |\psi_n\rangle + E_n \frac{\partial}{\partial\lambda}\langle\psi_n| |\psi_n\rangle = \langle\psi_n| \frac{\partial H}{\partial\lambda} |\psi_n\rangle$

Griffth 6.33

(a) Use $\lambda = e$ in the Feynman-Hellmann theorem to obtain $< 1/r >$.

$\frac{\partial E_n}{\partial e} = \frac{-me^3}{8\pi^2\epsilon_0^2\hbar^2(j_{max}+l+1)^2} = \frac{4E_n}{e}$

$\frac{\partial H}{\partial e} = -\frac{2e}{4\pi\epsilon_0 r}$, Feynman-Hellmann theorem then becomes $\frac{4E_n}{e} = \langle\psi_n|\frac{-2e}{4\pi\epsilon_0 r}|\psi_n\rangle$

$\Longrightarrow < \frac{1}{r} > = \frac{1}{an^2}$, where $a = \frac{4\pi\epsilon_0\hbar^2}{me^2}$

(b)Using the same way, $\frac{\partial E_n}{\partial l} = \frac{me^4}{16\pi^2\epsilon_0^2\hbar^2(j_{max}+l+1)^3} = -\frac{2E_n}{n}$

$\frac{\partial H}{\partial l} = \frac{\hbar^2(2l+1)}{2mr^2}$

$\Longrightarrow < \frac{1}{r^2} > = \frac{1}{a^2n^3(l+\frac{1}{2})}$