Notes for Quantum Mechanics

Richard Seto

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Perturbation theory: Anharmonic Oscillator

The stanadard problem has a hamiltoniun $\hat{H}_0$ which we can solve exactly, e.g. for the SHO its $\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}\,\mathrm{m}\omega^2\,\hat{x}^2$

Added to this is some sort of small perturbation $\hat{H}'$ which in the case on an anharmonic oscillator like a pendulum is $a\,\hat{x}^4$. So for our example the final Hamiltonian is $\hat{H}=\hat{H}_0+\hat{H}' = \frac{\hat{p}^2}{2m} + \frac{1}{2}\,\mathrm{m}\omega^2\,\hat{x}^2 + k\,\hat{x}^4$ where k is some constant..

It had better be small if perturbation theory is to work. In fact $k << \frac{1}{2}\mathrm{m}\omega^2$.

$\hat{x}=\sqrt{\frac{\hbar}{2\,\mathrm{m}\omega}}\,(\hat{a}^\dagger + \hat{a})$ $\hat{a}^\dagger|\mathrm{n}\rangle=\sqrt{n+1}\,|\mathrm{n+1}\rangle$ $\hat{a}|\mathrm{n}\rangle=\sqrt{n}\,|\mathrm{n-1}\rangle$ $E_n^{(0)} = \left(n+\frac{1}{2}\right)\hbar\omega$ and as usual we know the ground states $\hat{H}_0\,|n\rangle = E_n|\mathrm{n}\rangle$ (we will forget about the superscript (0) here. All states are the ground state.

Lets figure out the first order correction to the energy

$\hat{H}' = k\,\hat{x}^4 = k\left(\frac{\hbar}{2\,\mathrm{m}\omega}\right)^2 (\hat{a}^\dagger + \hat{a})^4$

we need to find $E_n^{(1)}=\hat{H}_{\mathrm{nn}}' = \langle n\,|\,\hat{H}'\,|n\rangle = k\left(\frac{\hbar}{2\,\mathrm{m}\omega}\right)^2 \langle n\,|\,(\hat{a}^\dagger + \hat{a})^4\,|n\rangle$ so the hard part now is evaluating $\langle n\,|\,(\hat{a}^\dagger + \hat{a})^4\,|n\rangle$

The only terms which give a non-zero value are the ones where three is the same number of raising and lowering operators. (remember 1; 121; 1331; 14**6**41) So there are 6. When you multiply out the term there are 4 a's or $\hat{a}^\dagger$'s in a row. They are $\hat{a}^\dagger\,\hat{a}^\dagger\,\hat{a}\,\hat{a}$, $\hat{a}^\dagger\,\hat{a}\,\hat{a}^\dagger\,\hat{a}$, $\hat{a}^\dagger\,\hat{a}\,\hat{a}\,\hat{a}^\dagger$, $\hat{a}\,\hat{a}^\dagger\,\hat{a}^\dagger\,\hat{a}$, $\hat{a}\,\hat{a}^\dagger\,\hat{a}\,\hat{a}^\dagger$, $\hat{a}\,\hat{a}\,\hat{a}^\dagger\,\hat{a}^\dagger$. We need sandwitch these between $|\mathrm{n}\rangle$'s

Note: in these sets, the second row gives what the value inside the $|\rangle$ should be, the third row gives the value of the coefficient afer operating with the raising or lowerin operator.

$$\left.\begin{array}{cccc} \hat{a}^\dagger & \hat{a}^\dagger & \hat{a} & \hat{a} \\ n & n-1 & n-2 & n-1 \\ \sqrt{n} & \sqrt{n-1} & \sqrt{n-1} & \sqrt{n} \end{array}\right) = n(n-1) = n^2 - n$$

$$\left.\begin{array}{cccc} \hat{a}^\dagger & \hat{a} & \hat{a}^\dagger & \hat{a} \\ n & n-1 & n & n-1 \\ \sqrt{n} & \sqrt{n} & \sqrt{n} & \sqrt{n} \end{array}\right) = n^2 = n^2$$

$$\left.\begin{array}{cccc} \hat{a}^\dagger & \hat{a} & \hat{a} & \hat{a}^\dagger \\ n & n-1 & n & n+1 \\ \sqrt{n} & \sqrt{n} & \sqrt{n+1} & \sqrt{n+1} \end{array}\right) = n(n+1) = n^2 + n$$

$$\left.\begin{array}{cccc} \hat{a} & \hat{a}^\dagger & \hat{a}^\dagger & \hat{a} \\ n & n+1 & n & n-1 \\ \sqrt{n+1} & \sqrt{n+1} & \sqrt{n} & \sqrt{n} \end{array}\right) = n(n+1) = n^2 + n$$

$$\left.\begin{array}{cccc} \hat{a} & \hat{a}^\dagger & \hat{a} & \hat{a}^\dagger \\ n & n+1 & n & n+1 \\ \sqrt{n+1} & \sqrt{n+1} & \sqrt{n+1} & \sqrt{n+1} \end{array}\right) = (n+1)^2 = n^2 + 2\,n{+}1$$

$$\left.\begin{array}{cccc} \hat{a} & \hat{a} & \hat{a}^\dagger & \hat{a}^\dagger \\ n & n+1 & n+2 & n+1 \\ \sqrt{n+1} & \sqrt{n+2} & \sqrt{n+2} & \sqrt{n+1} \end{array}\right) = (n+2)\,(n+1) = n^2 + 3\,n + 2$$

Adding all the terms together gives $6\,n^2 + 6\,n + 3 = 3\,(2\,n^2 + 2\,n + 1)$

the final correction term is

$E_n{}^{(1)}$=k$\left(\frac{\hbar}{2\,\mathrm{m}\omega}\right)^2 3\,(2\,n^2 + 2\,n + 1)$=6k$\left(\frac{\hbar}{2\,\mathrm{m}\omega}\right)^2\left(n^2 + n + \frac{1}{2}\right)$

$E_n = \left(n + \frac{1}{2}\right)\hbar\omega + 6\,k\left(\frac{\hbar}{2\,\mathrm{m}\omega}\right)^2\left(n^2 + n + \frac{1}{2}\right)$

