PHYS 4302
Homework 1

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Problem 1 - Comparing exact and perturbative solutions

Consider a 1D harmonic oscillator problem, where the perturbation V causes a modification of the oscillator frequency:

$$H = H_0 + V, \quad H_0 = \frac{p^2}{2m} + \frac{Kx^2}{2} \tag{1}$$

$$V = \frac{K_1 x^2}{2}, \quad K_1 + K > 0. \tag{2}$$

Of course, this problem is trivially solved exactly yielding the oscillator solutions with a new frequency.

(a) Show that corrections to the nth energy level as calculated within the perturbation theory indeed correspond to the exact result, restricting yourselves to terms up to the second order in the perturbation. That is, compare exact and perturbative results with the accuracy $\propto K_1^2$.

$$E_n^0 = \left(n + \frac{1}{2}\right)\hbar\omega, \quad \omega = \sqrt{\frac{k}{m}}$$
$$|\Psi_n^0\rangle = |n\rangle, \ \ n \in \mathbb{N}$$

1st order correction:

$$E_n^{(1)} = \langle \psi_n^{(0)} | V | \psi_n^{(0)} \rangle = \langle n | V | n \rangle = \frac{K_1}{2} \langle n | x^2 | n \rangle = \boxed{\frac{K_1 \hbar}{4m\omega}(2n+1)}$$

2nd order correction:

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_- + a_+)$$

$$
\begin{aligned}
E_n^{(2)} &= \sum_{m\neq n} \frac{\left|\langle \psi_m^{(0)}|V|\psi_n^{(0)}\rangle\right|^2}{E_n^{(0)}-E_m^{(0)}} = \sum_{m\neq n} \frac{\left|\langle m|V|n\rangle\right|^2}{E_n^{(0)}-E_m^{(0)}} = \frac{K_1^2}{4}\sum_{m\neq n} \frac{\left|\langle m|x^2|n\rangle\right|^2}{E_n^{(0)}-E_m^{(0)}} \\
&= \frac{K_1^2}{4}\sum_{m\neq n} \frac{\left|\langle m|a_+^2+a_-^2+a_-a_++a_+a_-|n\rangle\right|^2}{E_n^{(0)}-E_m^{(0)}}\left(\frac{\hbar^2}{4m^2\omega^2}\right) \\
&= \frac{K_1^2}{4}\sum_{m\neq n} \frac{\left|\langle m|a_+^2|n\rangle+\langle m|a_-^2|n\rangle+\langle m|a_-a_+|n\rangle+\langle m|a_+a_-|n\rangle\right|^2}{E_n^{(0)}-E_m^{(0)}}\left(\frac{\hbar^2}{4m^2}\right)
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{K_1^2\hbar^2}{16m^2\omega^2}\left(\frac{(n+1)(n+2)\langle n+2|n+2\rangle}{E_n^{(0)}-E_{n+2}^{(0)}}+\frac{n(n-1)\langle n-2|n-2\rangle}{E_n^{(0)}-E_{n-2}^{(0)}}\right) \\
&= \frac{K_1^2\hbar^2}{16m^2\omega^2}\left(\frac{n^2+3n+2}{-2\hbar\omega}+\frac{n^2-n}{2\hbar\omega}\right) = \frac{K_1^2\hbar^2}{16m^2\omega^2}\left(\frac{1}{2\hbar\omega}\right)\left(-n^2-3n-2+n^2-n\right) \\
&= \boxed{-\frac{K_1^2\hbar}{16m^2\omega^3}(2n+1)}
\end{aligned}
$$

Exact solution:

$$
H = H_0 + V = \frac{p^2}{2m}+\frac{Kx^2}{2}+\frac{K_1x^2}{2} = \frac{p^2}{2m}+\frac{x^2(K+K_1)}{2}
$$

$$
E_n = \left(n+\frac{1}{2}\right)\hbar W
$$

$$
\begin{aligned}
W &= \sqrt{\frac{K+K_1}{m}} = \sqrt{\frac{K}{m}}\sqrt{1+\frac{K_1}{K}} = \omega\sqrt{1+\frac{K_1}{K}} \\
&= \omega\left(1+\frac{K_1}{2K}-\frac{K_1^2}{8}+\cdots\right) \\
E_n &= \left(n+\frac{1}{2}\right)\hbar\left(\omega+\frac{\omega K_1}{2K}-\frac{\omega K_1^2}{8K^2}+\cdots\right) \\
&= \left(\frac{2n+1}{2}\right)\hbar\omega+\frac{K_1\hbar\omega}{4m\omega K}(2n+1)-\frac{(2n+1)\hbar\omega K_1^2}{16K^2} \\
&= E_n^{(0)}+\boxed{\frac{K_1\hbar}{4m\omega}(2n+1)}+\boxed{-\frac{(2n+1)K_1^2\hbar}{16m^2\omega^3}}+\cdots
\end{aligned}
$$

(b) Specify the condition for the validity of the perturbative treatment. – When specifying applicability conditions like $A \ll B$ or $A/B \ll 1$, it ordinarily suffices to use only symbols of system parameters without explicitly writing numerical factors on the order of 1, such as, e.g. in $\sqrt{3}A \ll B$, where $\sqrt{3} \sim 1$. Depending on specifics, larger numerical factors like, e.g., 2π or π^2 may be featured. Also helpful for understanding is to use physically meaningful combinations of parameters, comparing, e.g., certain energy or length scales.

Perturbations must be very small in comparison to the original state of the system in order for perturbation theory corrections to be valid, so $\boxed{H_0 \gg v}$.

Problem 2

Consider a 1D anharmonic oscillator problem:

$$H = H_0 + V, \quad H_0 = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \tag{3}$$

$$V = \lambda x^4, \quad \lambda > 0. \tag{4}$$

There is no exact solution in this case.

(a) Treat V in Eq. (4) perturbatively and find the corrections to the *ground state* energy up to the second order (that is, with accuracy $\propto \lambda^2$).

$$E_n^{(0)} = \left(n + \frac{1}{2}\right)\hbar\omega$$

1st order correction:

$$E_n^{(1)} = \langle\psi_n^{(0)}|V|\psi_n^{(0)}\rangle = \langle n|V|n\rangle = \lambda\langle n|x^4|n\rangle = \boxed{\frac{3\lambda\hbar^2}{2m^2\omega^2}(2n+1)}$$

2nd order correction:

$$\begin{aligned}
E_n^{(2)} &= \sum_{m\neq n} \frac{\left|\langle\psi_m^{(0)}|V|\psi_n^{(0)}\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}} = \sum_{m\neq n} \frac{\left|\langle m|V|n\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}} \\
&= \lambda^2 \sum_{m\neq n} \frac{\left|\langle m|\left(a_+^2 + a_-^2 + a_-a_+ + a_+a_-\right)^2|n\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}} \\
&= \lambda^2 \sum_{m\neq n} \frac{\left|\langle m|a_-^4 + a_-^2a_+a_- + a_-^3a_+ + a_-a_+a_-^2|n\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}} \\
&= \lambda^2 \sum_{m\neq n} \frac{\langle m|a_-^4|n\rangle}{E_n^{(0)} - E_m^{(0)}} + \frac{\langle m|a_-^2a_+a_-|n\rangle}{E_n^{(0)} - E_m^{(0)}} + \cdots \\
&= \lambda^2\left(\frac{12}{\hbar\omega} + \frac{6}{\hbar\omega}\right) = \boxed{\frac{18\lambda^2}{\hbar\omega}}
\end{aligned}$$

(b) Specify the condition for the validity of the low-order perturbation theory and represent it using physically meaningful quantities.

Perturbations must be very small in comparison to the original state of the system in order for perturbation theory corrections to be valid, so $\boxed{H_0 \gg v}$.

Problem 3

In this problem you are asked to evaluate certain very useful expectation values by using Feynman-Hellman's theorem (and learning to appreciate its powerful convenience):

$$\langle n|\frac{\partial H(\lambda)}{\partial\lambda}|n\rangle = \frac{\partial E_n(\lambda)}{\partial\lambda}. \tag{5}$$

In expression (5), $H(\lambda)$ is the parameter $\lambda -$ dependent system Hamiltonian and $|n\rangle$ is a generically labeled stationary state: $H(\lambda)|n\rangle = E_n(\lambda)|n\rangle$.

We will now turn from the generic description to a specific problem of the (non-relativistic) Hydrogen atom, where it is customary to denote stationary discrete states as $|nlm\rangle$ by specifying three quantum numbers. Recall that the principal quantum number $n = 1, 2, \ldots$ is actually "constructed" of the independent radial quantum number $n_r = 1, 2, \ldots$ and angular momentum (number) $l = 0, 1, 2\ldots$:

$$n = n_r + l. \tag{6}$$

It is the principal quantum number combination that determines the energies of the $|nlm\rangle$ states:

$$E_{nlm} = E_n = -\frac{Ry}{n^2}. \tag{7}$$

In addition to the energy scale $Ry = k_e^2 mq^4/2\hbar^2$, the Hydrogen atom problem yields the length scale $a_B = \hbar^2/k_e mq^2$ (here m is of course the electron mass, not the magnetic quantum number!).

Inspect the Schrödinger equation for the radial wave function in the Hydrogen atom problem and find the appropriate parametric dependencies in order to use the generic Eq. (5) for the following:

(a) Prove that the expectation value of the inverse distance to the nucleus, $1/r$:

$$\langle nlm|\frac{1}{r}|nlm\rangle = \frac{1}{n^2 a_B}. \tag{8}$$

Using the radial Hamiltonian for Hydrogen and its solved eigenvalues:

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \\ E_n &= -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2\left(j_{\max}+l+1\right)^2} \end{aligned}$$

$$\begin{aligned} \frac{\partial E_n}{\partial e} &= \frac{-4me^3}{32\pi^2\epsilon_0^2\hbar^2\left(j_{\max}+l+1\right)^2} \\ &= \frac{-4me^4}{e\left(32\pi^2\epsilon_0^2\hbar^2\left(j_{\max}+l+1\right)^2\right)} = \frac{4}{e}E_n \\ \frac{\partial H}{\partial e} &= -\frac{e}{2\lambda\epsilon_0 r} \\ \frac{\partial E_n}{\partial e} &= \langle nlm|\frac{\partial H}{\partial e}|nlm\rangle \to \frac{4}{e}E_n = \langle nlm| - \frac{e}{2\pi\epsilon_0 r}|nlm\rangle \\ \langle\frac{1}{r}\rangle &= \langle nlm|\frac{1}{r}|nlm\rangle = -\frac{8\pi\epsilon_0}{e^2}E_n = \left(-\frac{8\pi\epsilon_0}{e^2}\right)\left(-\frac{e^2}{8\pi\epsilon_0 a_B n^2}\right) = \boxed{\frac{1}{n^2 a_B}} \end{aligned}$$

(b) Prove that the expectation value of the square of the inverse distance to the nucleus, $1/r^2$:

$$\langle nlm|\frac{1}{r^2}|nlm\rangle = \frac{1}{n^3\left(l+\frac{1}{2}\right)a_B^2}. \tag{9}$$

$$\begin{aligned}
\frac{\partial E_n}{\partial l} &= \frac{2me^4}{32\pi^2\epsilon_0^2\hbar^2\left(j_{\max}+l+1\right)^3} = -\frac{2E_n}{n} \\
\frac{\partial H}{\partial l} &= \frac{\hbar^2}{2mr^2}\left(2l+1\right) \\
\frac{\partial E_n}{\partial l} = \langle nlm|\frac{\partial H}{\partial l}|nlm\rangle \\
-\frac{2E_n}{n} &= \langle nlm|\frac{\hbar^2}{2mr^2}\left(2l+1\right)|nlm\rangle \\
\langle\frac{1}{r^2}\rangle &= \langle nlm|\frac{1}{r^2}|nlm\rangle = -\frac{4mE_n}{\hbar^2 n\left(2l+1\right)} \\
&= \frac{4m}{\hbar^2 n\left(2l+1\right)}\left(\frac{1}{\hbar}\frac{e^2}{4\pi\epsilon_0}\frac{1}{n^2 a_B}\right) \\
&= \boxed{\frac{1}{\left(l+\frac{1}{2}\right)n^3 a_B^2}}, \text{ given } a_B^2 = \frac{4\pi\epsilon_0\hbar^2}{me^2}
\end{aligned}$$

After you master "tricks" of the usage of Eq. (5), ask yourself if you would instead prefer the actual integration with the respective explicit wave functions in calculating (8) and (9).