

Practice perturbing the quantum harmonic oscillator

Problem statement: Consider a one-dimensional quantum harmonic oscillator; that is, consider a particle with the following Hamiltonian:

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2. \quad (1)$$

Now, perturb the Hamiltonian as $\hat{H} \rightarrow \hat{H} + \hat{H}'$ where,

$$\hat{H}' = \epsilon\hat{x}. \quad (2)$$

Solve for eigenstates and energies exactly and using time-independent perturbation theory to second order for the energies and first order for the states.

A useful reminder: The (unperturbed) Harmonic oscillator energy eigenstates, $|\psi_n^{(0)}\rangle$ in the position representation are,

$$\psi_n^{(0)} = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2/2} H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right), \quad (3)$$

and the (unperturbed) energy eigenvalues are,

$$E_n^{(0)} = \hbar\omega\left(n + \frac{1}{2}\right). \quad (4)$$

We can simplify computations using ladder operators,

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right), \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right), \quad (5)$$

which obey the relations,¹

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}), \quad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}^\dagger - \hat{a}), \quad (6)$$

and act on the energy eigenstates as,

$$\hat{a}|\psi_n^{(0)}\rangle = \sqrt{n}|\psi_{n-1}^{(0)}\rangle, \quad \hat{a}^\dagger|\psi_n^{(0)}\rangle = \sqrt{n+1}|\psi_{n+1}^{(0)}\rangle, \quad \hat{a}|\psi_0^{(0)}\rangle = 0. \quad (7)$$

This saves us from having to do integrals like this:

$$\langle\psi_0^{(0)}|\hat{x}|\psi_1^{(0)}\rangle = \int_{-\infty}^{\infty} dx \psi_0^{(0)}(x)^* x \psi_1^{(0)}(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \sqrt{2\pi} \left(\frac{m\omega}{\hbar\pi}\right)^{3/4} \int_{-\infty}^{\infty} dx x e^{-\frac{m\omega}{2\hbar}x^2} x e^{-\frac{m\omega}{2\hbar}x^2} = \sqrt{\frac{\hbar}{2m\omega}}, \quad (8)$$

which I actually did in *Mathematica*:

$$\text{In}[1]:= \sqrt{2\pi}\left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \left(\frac{m\omega}{\hbar\pi}\right)^{3/4} \text{Integrate}\left[x e^{-\frac{m\omega}{2\hbar}x^2} x e^{-\frac{m\omega}{2\hbar}x^2}, \{x, -\infty, \infty\}, \text{Assumptions} \rightarrow \omega > 0 \ \&\& \hbar > 0 \ \&\& m > 0\right]$$

$$\text{Out}[1]= \sqrt{\frac{\hbar}{2m\omega}}$$

¹There was previously a typo in line 6; \hat{p} had the wrong units! It is now corrected. My apologies.

Instead, we do this:

$$\begin{aligned}
\langle \psi_0^{(0)} | \hat{x} | \psi_1^{(0)} \rangle &= \langle \psi_0^{(0)} | \hat{x} | \psi_1^{(0)} \rangle = \langle \psi_0^{(0)} | \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger + \hat{a}) | \psi_1^{(0)} \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle \psi_0^{(0)} | (\hat{a}^\dagger | \psi_1^{(0)} \rangle + \hat{a} | \psi_1^{(0)} \rangle) \\
&= \sqrt{\frac{\hbar}{2m\omega}} \langle \psi_0^{(0)} | (\sqrt{1+1} | \psi_{1+1}^{(0)} \rangle + \sqrt{1} | \psi_{1-1}^{(0)} \rangle) = \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{2} \langle \psi_0^{(0)} | \psi_2^{(0)} \rangle + \langle \psi_0^{(0)} | \psi_0^{(0)} \rangle) \\
&= \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{2} \times 0 + 1) = \sqrt{\frac{\hbar}{2m\omega}},
\end{aligned} \tag{9}$$

which agrees with the integral. Note that in the last line, we used that the energy eigenstates form an orthonormal basis,

$$\langle \psi_n^{(0)} | \psi_m^{(0)} \rangle = \delta_{n,m}, \tag{10}$$

where δ_{nm} is the Kronecker delta symbol. **At any point in this computation, we could replace one of the bra-ket expressions with an integral and obtain the same results.** ²

Perturbative solution: Write the Hamiltonian as $\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$ and the perturbing Hamiltonian as $\hat{H}' = \epsilon\sqrt{\hbar/(2m\omega)}(\hat{a}^\dagger + \hat{a})$. We compute the perturbed energies as:

$$\begin{aligned}
E_n^{(1)} &= \langle \psi_n^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle = \epsilon\sqrt{\frac{\hbar}{2m\omega}} \langle \psi_n^{(0)} | (\hat{a} + \hat{a}^\dagger) | \psi_n^{(0)} \rangle = \epsilon\sqrt{\frac{\hbar}{2m\omega}} \langle \psi_n^{(0)} | (\hat{a} + \hat{a}^\dagger) | \psi_n^{(0)} \rangle \\
&= \epsilon\sqrt{\frac{\hbar}{2m\omega}} \langle \psi_n^{(0)} | (\sqrt{n} | \psi_{n-1}^{(0)} \rangle + \sqrt{n+1} | \psi_{n+1}^{(0)} \rangle) = \epsilon\sqrt{\frac{\hbar}{2m\omega}} (\sqrt{n}\delta_{n,n-1} + \sqrt{n+1}\delta_{n,n+1}) = 0.
\end{aligned} \tag{11}$$

The first-order corrections are zero. The first-order corrections to the stationary states are,

$$\begin{aligned}
| \psi_n^{(1)} \rangle &= \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} | \psi_m^{(0)} \rangle = \epsilon\sqrt{\frac{\hbar}{2m\omega}} \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | \hat{a}^\dagger + \hat{a} | \psi_n^{(0)} \rangle}{\hbar\omega(\frac{1}{2} + n - \frac{1}{2} - m)} | \psi_m^{(0)} \rangle \\
&= \epsilon\sqrt{\frac{\hbar}{2m\omega}} \sum_{m \neq n} \frac{\sqrt{n+1} \langle \psi_m^{(0)} | \psi_{n+1}^{(0)} \rangle + \sqrt{n} \langle \psi_m^{(0)} | \psi_{n-1}^{(0)} \rangle}{n-m} | \psi_m^{(0)} \rangle = \epsilon\sqrt{\frac{\hbar}{2m\omega}} \sum_{m \neq n} \frac{\sqrt{n+1}\delta_{m,n+1} + \sqrt{n}\delta_{m,n-1}}{n-m} | \psi_m^{(0)} \rangle \\
&= \epsilon\sqrt{\frac{\hbar}{2m\omega}} \left[0 + \dots + 0 + \frac{\sqrt{n+1}\delta_{n-1,n+1} + \sqrt{n}\delta_{n-1,n-1}}{n-(n-1)} | \psi_{n-1}^{(0)} \rangle + \frac{\sqrt{n+1}\delta_{n+1,n+1} + \sqrt{n}\delta_{n+1,n-1}}{n-(n+1)} | \psi_{n+1}^{(0)} \rangle + 0 + \dots + 0 \right] \\
&= \epsilon\sqrt{\frac{\hbar}{2m\omega}} (\sqrt{n} | \psi_{n-1}^{(0)} \rangle - \sqrt{n+1} | \psi_{n+1}^{(0)} \rangle).
\end{aligned} \tag{12}$$

This makes our first-order perturbed energy eigenstates:

$$| \psi_n^{\text{1st order}} \rangle = | \psi_n^{(0)} \rangle + | \psi_n^{(1)} \rangle = | \psi_n^{(0)} \rangle + \epsilon\sqrt{\frac{\hbar}{2m\omega}} (\sqrt{n} | \psi_{n-1}^{(0)} \rangle - \sqrt{n+1} | \psi_{n+1}^{(0)} \rangle). \tag{13}$$

The second-order corrections to the energies are computed very similarly to the first-order corrections to the stationary states:

$$\begin{aligned}
E_n^{(2)} &= \sum_{m \neq n} \frac{|\langle \psi_m^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}} = \frac{\epsilon^2}{2m\omega^2} \sum_{m \neq n} \frac{|\langle \psi_m^{(0)} | \hat{x} | \psi_n^{(0)} \rangle|^2}{n-m} = \frac{\epsilon^2}{2m\omega^2} \sum_{m \neq n} \frac{|\langle \psi_m^{(0)} | \hat{a} + \hat{a}^\dagger | \psi_n^{(0)} \rangle|^2}{n-m} \\
&= \frac{\epsilon^2}{2m\omega^2} \sum_{m \neq n} \frac{|\sqrt{n} \langle \psi_m^{(0)} | \psi_{n-1}^{(0)} \rangle + \sqrt{n+1} \langle \psi_m^{(0)} | \psi_{n+1}^{(0)} \rangle|^2}{n-m} = \frac{\epsilon^2}{2m\omega^2} \sum_{m \neq n} \frac{|\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}|^2}{n-m} \\
&= \frac{\epsilon^2}{2m\omega^2} \left[0 + \dots + 0 + \frac{|\sqrt{n}\delta_{n-1,n-1} + \sqrt{n+1}\delta_{n-1,n+1}|^2}{n-(n-1)} + \frac{|\sqrt{n}\delta_{n+1,n-1} + \sqrt{n+1}\delta_{n+1,n+1}|^2}{n-(n+1)} + 0 + \dots + 0 \right] \\
&= \frac{\epsilon^2}{2m\omega^2} [|\sqrt{n}|^2 - |\sqrt{n+1}|^2] = -\frac{\epsilon^2}{2m\omega^2}.
\end{aligned} \tag{14}$$

To second order, the perturbed energies are,

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right) - \frac{\epsilon^2}{2m\omega^2} + O(\epsilon^3). \tag{15}$$

²There is something tricky in notation here: m is the symbol for both an index and the mass. It should hopefully be clear from context which is which, but be aware that this notational clash exists.

Exact solution: Observe that if we shift the potential by x_0 , we have,

$$\frac{1}{2}m\omega^2(x - x_0)^2 = \frac{1}{2}m\omega^2x^2 - m\omega^2x_0x + \frac{1}{2}m\omega^2x_0^2, \quad (16)$$

so we can reproduce the perturbed potential using $\epsilon = -m\omega^2x_0 \implies x_0 = -\epsilon/(m\omega^2)$ up to an overall constant:

$$\frac{1}{2}m\omega^2\left(x + \frac{\epsilon}{m\omega^2}\right)^2 = \frac{1}{2}m\omega^2x^2 + \epsilon x + \frac{\epsilon^2}{2m\omega^2}. \quad (17)$$

As \hat{p} is remains invariant under the transformation $x \rightarrow x - x_0$, we can write,

$$\hat{H} + \hat{H}' = \hat{H}\Big|_{x \rightarrow x + \epsilon/(m\omega^2)} - \frac{\epsilon^2}{2m\omega^2}, \quad (18)$$

where $\hat{H}\Big|_{x \rightarrow x + \epsilon/(m\omega^2)}$ is the Hamiltonian with the x -coordinate shifted. The stationary states of $\hat{H}\Big|_{x \rightarrow x + \epsilon/(m\omega^2)}$ are the stationary states of \hat{H} , shifted by $-\epsilon/(m\omega^2)$, and shifting the Hamiltonian by a constant does not change the eigenstates (up to a phase). Therefore, the eigenstates of $\hat{H} + \hat{H}'$ are the usual QHO eigenfunctions, shifted by $-\epsilon/(m\omega^2)$, and the energy eigenvalues are those of the QHO, shifted by $-\epsilon^2/(2m\omega^2)$, so the energy eigenvalues are $E_n = \hbar\omega(n + \frac{1}{2}) - \epsilon^2/(2m\omega^2)$. This shows that the perturbative expansion of the energy eigenvalues is exact to second order!