CAS PY 452 — Quantum Physics II

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Discussion Notes
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Practice perturbing the quantum harmonic oscillator

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

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

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

$$\hat{H}' = \epsilon\hat{x}. \tag{2}$$

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,

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

where H_n are the Hermite polynomials, and the (unperturbed) energy eigenvalues are,

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

We can simplify computations using ladder operators,

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

which obey the relations,[1]

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

and act on the energy eigenstates as,

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

This saves us from having to do integrals like this:

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

which I actually did in *Mathematica*:

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

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

[1] There was previously a typo in line 6. It is now corrected. My apologies.

Instead, we do this:

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

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,

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

This makes our first-order perturbed energy eigenstates:

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

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

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

To second order, the perturbed energies are,

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

[2] There 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,

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

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:

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

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

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

where $\hat{H}\Big|_{x\to x+\epsilon/(m\omega^2)}$ is the Hamiltonian with the x-coordinate shifted. The stationary states of $\hat{H}\Big|_{x\to x+\epsilon/(m\omega^2)}$ 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!