Some Perturbation Problems from Quantum Mechanics

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This time we shall discuss some problems of time-independent perturbation in Quantum Mechanics. We consider ‘slightly modified’ harmonic oscillators and find energy eigenvalues by perturbation method, and also by exact treatment, for comparison. The reader should not form the impression that it can be done with every problem! Indeed, perturbation method is an approximate method for solving problems which cannot be solved exactly. A careful study of these problems will also help develop a good understanding of the use of ladder operators in Quantum Mechanics.

Q1 Consider a 1D harmonic oscillator with potential energy $V = \frac{1}{2}(1 + \epsilon)kx^2$, where $k$, $\epsilon$ are constants.

(a) Find the expression for exact energy eigenvalues. Expand an arbitrary eigenvalue in a power series in $\epsilon$ upto to second power.

(b) Now obtain the energy eigenvalues by treating the term $\frac{1}{2}\epsilon kx^2 = \epsilon V$ as a small perturbation (i.e, $\epsilon \ll 1$, and dimensionless). Show that the perturbation calculations give the same results as the exact treatment of part (a) upto second order in $\epsilon$.

Solution

(a) We shall assume the solution for the standard 1D harmonic oscillator with potential energy term $V = \frac{1}{2}kx^2$, where $k$ is the spring constant. As we know, the energy eigenvalues for this oscillator are given by $E_n = (n + \frac{1}{2})\hbar\omega$, with $n = 0, 1, 2, \ldots$, $\omega = \sqrt{k/m}$, $m$ being the mass. And if we take the given potential $V = \frac{1}{2}(1 + \epsilon)kx^2$, we can readily give it the standard form by simply setting $k' = (1 + \epsilon)k$, as $\epsilon$ is a constant. In this case we have the energy eigenvalues $E_n' = (n + \frac{1}{2})\hbar\omega'$, $\omega' = \sqrt{k'/m} = \sqrt{(1 + \epsilon)k/m} = \sqrt{(1 + \epsilon)\omega}$. Thus we have $E_n' = \sqrt{(1 + \epsilon)E_n}$. For $\epsilon < 1$ we expand this in powers of $\epsilon$ (Mclaurin series) as

$$E_n' = \left[ 1 + \frac{1}{2}\epsilon - \frac{1}{8}\epsilon^2 + \ldots \right] E_n$$

$$= E_n + \frac{1}{2}\epsilon E_n - \frac{1}{8}\epsilon^2 E_n + \ldots$$

(1)

(b) The Hamiltonian in this case is

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 + \frac{1}{2}\epsilon kx^2$$

$$= H_0 + H'$$

(2)

Where $H_0 = \frac{p^2}{2m} + \frac{1}{2}kx^2$ is the unperturbed Hamiltonian and $H' = \frac{1}{2}\epsilon kx^2$ is the perturbation term, with $\epsilon \ll 1$. The first order correction $E_n^{1}$ to the unperturbed energy $E_n$ is given by (note $E_n^{1}$ is different
from $E_n'$ of equation (1)!

$$E_n^1 = \langle \psi_n | H' | \psi_n \rangle$$

$$= \frac{1}{2} \epsilon k \langle \psi_n | x^2 | \psi_n \rangle$$

$$= \frac{1}{2} \epsilon k \langle n | x^2 | n \rangle$$

$$= \frac{1}{2} \epsilon m \omega^2 \langle n | x^2 | n \rangle$$

where $|\psi_n\rangle$ is the unperturbed eigenfunction for the eigenvalue $E_n$, and we have used the compact notation $|n\rangle$ for $|\psi_n\rangle$. The easiest way to evaluate the bracket term $\langle n | x^2 | n \rangle$ is to use the harmonic oscillator ladder operators $a_\pm$. The position operator $x$ is given by $x = \sqrt{\frac{\hbar}{2m\omega}} (a_+ + a_-)$, and so we have $x^2 = \frac{\hbar}{2m\omega} [a_+^2 + a_-^2 + a_+a_- + a_-a_+]$ (Remember that $a_+a_- \neq a_-a_+!$). Using this in the above equation

$$E_n^1 = \frac{1}{2} \epsilon m \omega^2 \cdot \frac{\hbar}{2m\omega} \langle n | [a_+^2 + a_-^2 + a_+a_- + a_-a_+] | n \rangle$$

$$= \frac{\hbar \omega}{4} \epsilon \langle n | [a_+^2 + a_-^2 + a_+a_- + a_-a_+] | n \rangle$$

We have $a_+ |n\rangle = \sqrt{n+1} |n+1\rangle$ and $a_- |n\rangle = \sqrt{n-1} |n-1\rangle$, and from these relations we readily get $a_+^2 |\psi_n\rangle = \sqrt{(n+1)(n+2)} |n+2\rangle$, $a_-^2 |\psi_n\rangle = \sqrt{n(n-1)} |n-2\rangle$, $a_+a_- |n\rangle = n |n\rangle$ and $a_-a_+ |n\rangle = (n+1) |n\rangle$. Using these in the above equation

$$E_n^1 = \frac{\hbar \omega}{4} \epsilon \langle n | \left[ \sqrt{(n+1)(n+2)} |n+2\rangle + \sqrt{n(n-1)} |n-2\rangle + n |n\rangle + (n+1) |n\rangle \right]$$

$$= \frac{\hbar \omega}{4} \epsilon [n+(n+1)]$$

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

$$E_n^1 = \frac{1}{2} \epsilon E_n$$

$$E_n^1 = \frac{1}{2} \epsilon E_n$$

(3)

In the above simplifications we have used the fact that the states $|n\rangle$ are orthonormal and therefore $\langle n | n+1 \rangle = \langle n | n+1 \rangle = 0$, and $\langle n | n \rangle = 1$. This correction term in equation (3) is the same as the term in the series in equation (1) (i.e., the first power of $\epsilon$ term).

The second order energy correction is given by

$$E_n^2 = \sum_{k \neq n} \frac{|\langle k | H' | n \rangle|^2}{E_n - E_k}$$

(4)

In the above equation the summation is over $k$ and the limits are $k = 0$ to $k = \infty$, excluding $k = n$, as indicated. In the rest of the article also this is to be understood. Now we have

$$|\langle k | H' | n \rangle|^2 = \frac{1}{4} \epsilon^2 m^2 \omega^4 \langle k | x^2 | n \rangle^2$$

$$= \frac{1}{4} \epsilon^2 m^2 \omega^4 \left| \langle k | x^2 | n \rangle \right|^2$$

$$= \frac{1}{4} \epsilon^2 m^2 \omega^4 \left| \frac{\hbar}{2m\omega} \langle k | [a_+^2 + a_-^2 + a_+a_- + a_-a_+] | n \rangle \right|^2$$

$$= \frac{1}{16} \epsilon^2 m^2 \omega^2 \left| \langle k | [a_+^2 + a_-^2 + a_+a_- + a_-a_+] | n \rangle \right|^2$$

(5)
Q2 Consider a charged particle in the 1D harmonic oscillator potential. Suppose the particle is placed in a weak, uniform electric field. (a) Treat the electric field as a small perturbation and obtain the first and second order corrections to harmonic oscillator energy eigenvalues. (b) Find the exact energy eigenvalues and compare them to the energies obtained in (a).

Solution

(a) Let us denote uniform electric field by \( E \) (we have to reserve \( E \) for energy). The corresponding potential energy is \( H' = -qE x \), where \( q \) is the charge. Thus the Hamiltonian for the charged particle is

\[
H = H_0 + H' = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 - qE x
\]  

Using equation (5) and \( E_k - E_n = (k - n) \hbar \omega \) in equation (4) we have

\[
E_n^2 = \frac{1}{16} \epsilon^2 \hbar^2 \sum_{k \neq n} \left[ \frac{\langle k | a_+^2 + a_+ a_- + a_- a_+ | n \rangle}{(n-k)} \right]^2
\]  

Now, \( \langle k | a_+^2 | n \rangle = (n+1)(n+2) \), as the states \( | n \rangle \) are orthonormal (Here \( \delta_{k,n+2} \) is the Kronecker delta). Similarly, \( \langle k | a_+ a_- | n \rangle = \sqrt{n(n-1)} \), \( | n \rangle \) and \( \langle k | a_- a_+ | n \rangle = (n+1)(n) \), because \( k \neq n \). Using all of this in equation (6) we have

\[
E_n^2 = \frac{1}{16} \epsilon^2 \hbar \omega \sum_{k \neq n} \frac{(n+1)(n+2) \delta_{k,n+2} + \sqrt{n(n-1)} \delta_{k,n-2}}{(n-k)}^2
\]  

In the above equation we expand the square term on RHS by using the facts that \( (\delta_{k,n+2})^2 = \delta_{k,n+2} \), \( (\delta_{k,n-2})^2 = \delta_{k,n-2} \) and \( \delta_{k,n+2} \cdot \delta_{k,n-2} = 0 \), and get

\[
E_n^2 = \frac{1}{16} \epsilon^2 \hbar \omega \left[ \sum_{k \neq n} \frac{(n+1)(n+2) \delta_{k,n+2}}{(n-k)} + \sum_{k \neq n} \frac{n(n-1) \delta_{k,n-2}}{(n-k)} \right]
\]  

In the above equation RHS, in the first sum all the terms except for which \( k = n+2 \) are zero (because of the presence of the Kronecker delta). Similarly, in the second sum all the terms except for which \( k = n-2 \) vanish. Thus we get

\[
E_n^2 = \frac{1}{16} \epsilon^2 \hbar \omega \left[ \frac{(n+1)(n+2)}{(n-n-2)} + \frac{n(n-1)}{(n+n+2)} \right]
\]  

\[
= -\frac{1}{8} \epsilon^2 \left( n + \frac{1}{2} \right) \hbar \omega
\]  

\[
= -\frac{1}{8} \epsilon^2 E_n
\]  

We can see that this second order perturbation correction to energy eigenvalue is also same as obtained in the exact solution of equation (1).
The first order correction to energy eigenvalue is

\[ E_n^1 = \langle \psi_n | H' | \psi_n \rangle \]
\[ = (n | (-q\mathcal{E}x) | n) \]
\[ = - q\mathcal{E} (n | x | n) \]
\[ = - q\mathcal{E} (n \sqrt{\frac{\hbar}{2m\omega}} | a_+ + a_- | n) \]
\[ = - q\mathcal{E} \cdot \sqrt{\frac{\hbar}{2m\omega}} \langle n | (a_+ + a_-) | n \rangle \]
\[ = - q\mathcal{E} \sqrt{\frac{\hbar}{2m\omega}} \left[ \sqrt{n + 1} \langle n | n + 1 \rangle + \sqrt{n} \langle n | n - 1 \rangle \right] \]
\[ = 0 \]

because \( \langle n | n + 1 \rangle = \langle n | n - 1 \rangle = 0 \), due to orthonormality. Thus the first order energy correction is zero.

Now we move on to calculate the second order correction. Please note that this calculation is very similar to the second order energy correction calculation done in Q1(b), and so we go right through with it without any interspersed explanations.

\[ E_n^2 = \sum_{k \neq n} \frac{|\langle k | H' | n \rangle|^2}{E_n - E_k} \]
\[ = \sum_{k \neq n} \frac{|\langle k | (-q\mathcal{E}x) | n \rangle|^2}{E_n - E_k} \]
\[ = \sum_{k \neq n} \frac{|(-q\mathcal{E}) | k | x | n \rangle|^2}{E_n - E_k} \]
\[ = q^2\mathcal{E}^2 \sum_{k \neq n} \frac{|\langle k | x | n \rangle|^2}{E_n - E_k} \]
\[ = q^2\mathcal{E}^2 \frac{\frac{\hbar}{2m\omega} \cdot \frac{1}{\hbar\omega} \cdot |\langle k | (a_+ + a_-) | n \rangle|^2}{(n - k)} \]
\[ = \frac{q^2\mathcal{E}^2}{2m\omega^2} \sum_{k \neq n} \frac{|\langle k | (a_+ + a_-) | n \rangle|^2}{(n - k)} \]
\[ = \frac{q^2\mathcal{E}^2}{2m\omega^2} \sum_{k \neq n} \frac{|\langle k | a_+ | n \rangle + \langle k | a_- | n \rangle|^2}{(n - k)} \]
\[ = \frac{q^2\mathcal{E}^2}{2m\omega^2} \sum_{k \neq n} \left[ \sqrt{n + 1} \langle k | n + 1 \rangle + \sqrt{n} \langle k | n - 1 \rangle \right]^2 \]
\[ = \frac{q^2\mathcal{E}^2}{2m\omega^2} \sum_{k \neq n} \left[ \sqrt{n + 1} \delta_{k,n+1} + \sqrt{n} \delta_{k,n-1} \right]^2 \]
\[ = \frac{q^2\mathcal{E}^2}{2m\omega^2} \sum_{k \neq n} \left[ (n + 1) \delta_{k,n+1} + n \delta_{k,n-1} \right] \]
\[ = \frac{q^2\mathcal{E}^2}{2m\omega^2} \left[ \sum_{k \neq n} \frac{(n + 1) \delta_{k,n+1}}{(n - k)} + \sum_{k \neq n} \frac{n \delta_{k,n-1}}{(n - k)} \right] \]
\[ E_n^2 = -\frac{q^2 E^2}{2m\omega^2} \left( \frac{n+1}{n-n-1} \cdot \frac{n}{n-n+1} \right) \]

That is quite a lot of work to get to \(-1\)!

(a) Now we find exact energy eigenvalues for the Hamiltonian given in equation (7). This problem we have already discussed on an earlier occasion in this column, but we present here once again for the sake of completeness. Also here it is slightly differently. For the Hamiltonian of equation (7) we have the Schrödinger time independent equation

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \left( \frac{1}{2}m\omega^2 x^2 - qE x \right) \psi = E \psi \]

The above equation can be transformed to the standard, simple harmonic oscillator equation with variable change \(x = y + \frac{qE}{m\omega^2}\). Since the term \(\frac{qE}{m\omega^2}\) is a constant, we have the double derivatives \(\frac{d^2 \psi}{dx^2} = \frac{d^2 \psi}{dy^2}\). With these substitutions, and a little algebra the above equation becomes

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dy^2} + \frac{1}{2}m\omega^2 y^2 \psi = \left( E + \frac{q^2 E^2}{2m\omega^2} \right) \psi = E' \psi \]

where \(E' = E + \frac{q^2 E^2}{2m\omega^2}\). The above equation is usual 1D harmonic oscillator, with energy eigenvalues \(E' = (n + \frac{1}{2}) \hbar\omega\). That gives us immediately the energy eigenvalues of the charged harmonic oscillator \(E = E' - \frac{q^2 E^2}{2m\omega^2}\). Thus, the correction to unperturbed harmonic oscillator energy is \(-\frac{q^2 E^2}{2m\omega^2}\), which is the same as we got with the perturbation method (equation (8)).