Chapter 6

6.1

Q. Suppose we put a delta-function bump in the center of the infinite square well:

\[ H' = \alpha \delta(x - a/2) \]  

where \( \alpha \) is a constant.

a)

Find the first-order correction to the allowed energies. Explain why the energies are not perturbed for even \( n \).

Sol:

For the infinite square well we have that the energies are given by:

\[ E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad n = 1, 2, 3 \ldots \]  

since each energy level is unique the spectrum is non-degenerate. So when we seek the first order corrections to the energy levels we can use non-degenerate perturbation theory:

\[ E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle \]

where \( \psi_n^0 \) are the unperturbed eigenfunctions of \( \hat{H} \). For the infinite square well these are:

\[ \psi_n^0(x) = \sqrt{\frac{2}{a}} \sin \left( \frac{n\pi}{a} x \right) . \]

Using eq.(3) we now get:

\[ E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle = \langle \psi_n^0 | \alpha \delta(x - a/2) | \psi_n^0 \rangle \]

\[ = \alpha \int_0^\infty (\psi_n^0(x))^* \delta(x - a/2) \psi_n^0(x) \, dx \]

\[ = \frac{2}{a} \cdot \alpha \int_0^\infty \sin \left( \frac{n\pi}{a} x \right) \delta(x - a/2) \sin \left( \frac{n\pi}{a} x \right) \, dx \]

\[ = \frac{2}{a} \cdot \alpha \sin^2 \left( \frac{n\pi}{a} \frac{a}{2} \right) = \begin{cases} 0 & \text{if } n \text{ = even} \\ \frac{2}{a} \cdot \alpha & \text{else} \end{cases} \]

For even \( n \) the correction is 0 at \( x = a/2 \). This is reasonable since the wave functions for even \( n \) are 0 (check it for at least one case!) where the delta-function is located - they are thus not affected by the perturbation.
b)

Find the first three nonzero terms in the expansion (eq.(6.13) in the text book) of the correction to the ground state \( \psi_1 \).

Sol:

Eq.(6.13) in the book is:

\[
\psi_n = \sum_{m \neq n} \frac{\langle \psi^0_m | H' | \psi^0_n \rangle}{E_n^0 - E_m^0} \psi_m^0 \quad \Rightarrow \quad \psi_1 = \sum_{m \neq 1} \frac{\langle \psi^0_m | H' | \psi^0_1 \rangle}{E_1^0 - E_m^0} \psi_m^0. \tag{5}
\]

First we evaluate \( \langle \psi^0_m | H' | \psi^0_1 \rangle \):

\[
\langle \psi^0_m | H' | \psi^0_1 \rangle = \int_0^a (\psi^0_m(x))^* \alpha \delta(x - \frac{a}{2}) \psi^0_1(x) \, dx
\]

\[= \alpha \int_0^a \sqrt{\frac{2}{a}} \sin \left( \frac{m\pi}{a} x \right) \sqrt{\frac{2}{a}} \sin \left( \frac{\pi}{a} x \right) \, dx = \alpha \frac{2}{a} \sin \left( \frac{m\pi}{2} \right) \sin \left( \frac{\pi}{2} \right) = \alpha \frac{2}{a} \sin \left( \frac{m\pi}{2} \right) \]

Now we insert this together with \( \psi_m^0 = \sqrt{\frac{2}{a}} \sin \left( \frac{m\pi}{a} x \right) \) into eq.(5):

\[
\psi_1(x) = \sum_{m \neq 1} \frac{\alpha \frac{2}{a} \sin \left( \frac{m\pi}{a} x \right)}{E_1^0 - E_m^0} \sqrt{\frac{2}{a}} \sin \left( \frac{m\pi}{a} x \right),
\]

we can now write out the first terms\(^1\) of the sum:

\[
\psi_1(x) = \alpha \left( \frac{2}{a} \right)^{3/2} \left[ \begin{array}{c} \frac{1}{E_1^0 - E_3^0} \sin \left( \frac{3\pi}{a} x \right) + \frac{1}{E_5^0 - E_3^0} \sin \left( \frac{5\pi}{a} x \right) + \frac{1}{E_7^0 - E_3^0} \sin \left( \frac{7\pi}{a} x \right) + \ldots \end{array} \right].
\]

Using eq.(2) for the energies and performing some basic algebra we obtain:

\[
\psi_1(x) = \sqrt{\frac{a}{2}} \frac{\alpha m}{\pi^2} \left[ \sin \left( \frac{2\pi}{a} x \right) - \frac{1}{3} \sin \left( \frac{2\pi}{a} x \right) + \frac{1}{5} \sin \left( \frac{2\pi}{a} x \right) + \ldots \right] \tag{6}
\]

\(^1\)Try to understand why they are \( m = 3, 5, 7 \).
6.2

Q. For the harmonic oscillator \[ V(x) = \frac{1}{2}kx^2 \], the allowed energies are:

\[ E_n = (n + 1/2)\hbar\omega \quad (n = 0, 1, 2, \ldots) \]  \hspace{1cm} (7)

where \( \omega = \sqrt{k/m} \) is the classical frequency. Now suppose the spring constant increases slightly: \( k \to (1 + \epsilon)k \).

a)

Q. Find the exact new energies. Expand your formula as a power series in \( \epsilon \), up to second order.

Sol:
The change in the spring constant also gives a change in the frequency:

\[ \tilde{k} = (1 + \epsilon)k \quad \Rightarrow \quad \tilde{\omega} = \sqrt{\frac{(1+\epsilon)k}{m}} = \sqrt{1 + \epsilon} \omega \]  \hspace{1cm} (8)

The new energies are obtained by using the new frequency \( \tilde{\omega} \):

\[ \tilde{E}_n = (n + \frac{1}{2})\hbar\tilde{\omega} = (n + \frac{1}{2})\hbar\omega \sqrt{1 + \epsilon}. \]  \hspace{1cm} (9)

Now make a power series expansion of this to second order in \( \epsilon \):

\[ \sqrt{1 + \epsilon} \approx 1 + \frac{1}{2}\epsilon - \frac{1}{8}\epsilon^2 + \ldots \]

to see that the new energies are approximately:

\[ \tilde{E}_n \approx (n + 1/2)\hbar\omega \left( 1 + \frac{1}{2}\epsilon - \frac{1}{8}\epsilon^2 + \ldots \right). \]  \hspace{1cm} (10)

b)

Q. Now calculate the first-order perturbation in energy using eq.(6.9) in the textbook. What is \( H' \) here? Compare your result with part (a). Hint: do not calculate any integral but use information from p.48-49 when suitable.

Sol:
The first-order energy perturbation is given by:

\[ E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle \]

and to calculate it we must know the perturbation \( H' \). For the Harmonic oscillator (in one dimension) we have the Hamiltonian:

\[ H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}kx^2 \]  \hspace{1cm} (11)
so with the new spring constant \( \tilde{k} = (1 + \epsilon)k \) we get:

\[
H + H' = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 + \frac{1}{2} \epsilon k x^2
\]

(12)

which gives us the first-order energy perturbation as:

\[
E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle = \frac{1}{2} \epsilon k \langle \psi_n^0 | x^2 | \psi_n^0 \rangle.
\]

From pages 48-49 in the text book we now find\(^2\)

\[
a^2 = \frac{\hbar}{2m\omega} \left[ a_+^2 + a_+ a_- + a_- a_+ + a_-^2 \right]
\]

(13)

Using eq.(13) the energy perturbation becomes:

\[
E_n^1 = \frac{1}{2} \epsilon k \frac{\hbar}{2m\omega} \langle \psi_n^0 | a_+^2 + a_+ a_- + a_- a_+ + a_-^2 | \psi_n^0 \rangle.
\]

(15)

\[
E_n^1 = \frac{1}{2} \epsilon k \frac{\hbar}{2m\omega} \left[ \langle \psi_n^0 | a_+^2 | \psi_n^0 \rangle + \langle \psi_n^0 | a_+ a_- | \psi_n^0 \rangle + \langle \psi_n^0 | a_- a_+ | \psi_n^0 \rangle + \langle \psi_n^0 | a_-^2 | \psi_n^0 \rangle \right]
\]

(16)

Now we will focus on the four scalar products:

\[
\langle \psi_n^0 | a_+^2 | \psi_n^0 \rangle + \langle \psi_n^0 | a_+ a_- | \psi_n^0 \rangle + \langle \psi_n^0 | a_- a_+ | \psi_n^0 \rangle + \langle \psi_n^0 | a_-^2 | \psi_n^0 \rangle
\]

let the first operator act on the ket (use eq.(14)) to give:

\[
\sqrt{n + 1} \langle \psi_n^0 | a_+ | \psi_{n+1}^0 \rangle + \sqrt{n} \langle \psi_n^0 | a_+ | \psi_{n-1}^0 \rangle + \sqrt{n + 1} \langle \psi_n^0 | a_- | \psi_{n+1}^0 \rangle + \sqrt{n} \langle \psi_n^0 | a_- | \psi_{n-1}^0 \rangle
\]

now let the remaining operator act on the new ket:

\[
\sqrt{n + 1} \sqrt{n + 2} \langle \psi_0^0 | \psi_{n+2}^0 \rangle + \sqrt{n} \sqrt{n + 1} \langle \psi_0^0 | \psi_{n+1}^0 \rangle + \sqrt{n + 1} \sqrt{n + 2} \langle \psi_n^0 | \psi_{n+2}^0 \rangle + \sqrt{n} \sqrt{n + 1} \langle \psi_n^0 | \psi_{n+1}^0 \rangle + \sqrt{n} \sqrt{n + 1} \langle \psi_n^0 | \psi_{n-1}^0 \rangle + \sqrt{n + 1} \sqrt{n + 2} \langle \psi_n^0 | \psi_{n-2}^0 \rangle
\]

\[
= 0 + n + (n + 1) + 0 = 2n + 1
\]

Inserting this into eq.(17) gives:

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

(17)

\[\text{Note: for } n = 0 \text{ the second and fourth scalar product should become 0 right after the first step, since } |\psi_{n-1}^0 \rangle \text{ does not exist. This is indeed also the case since } \sqrt{n} = \sqrt{0}.\]

\(^2\)There is a famous quote: "physics is just learning how to solve the harmonic oscillator problem at ever increasing level".
6.4

a)

Q. Find the second-order correction to the energies $E_n^2$ for the potential in problem 6.1. **Comment:** You can sum the series explicitly, obtaining $-2m(\alpha/\pi \hbar n)^2$ for odd $n$.

**Sol:**
The second-order energy correction (eq.(6.15) in the text book) is:

$$E_n^2 = \sum_{n \neq m} \frac{|\langle \psi_0^m | H' | \psi_0^n \rangle|^2}{E_n^0 - E_m^0}$$  \hspace{1cm} (18)

On p.2 in this chapter of solutions we found

$$\langle \psi_0^m | H' | \psi_0^n \rangle = \langle \psi_0^m | \alpha \delta(x - a/2) | \psi_0^n \rangle = \frac{2}{a} \cdot \alpha \sin \left( \frac{m\pi}{2} \right) \sin \left( \frac{n\pi}{2} \right)$$

so:

$$|\langle \psi_0^m | H' | \psi_0^n \rangle|^2 = \frac{4\alpha^2}{a^2} \sin^2 \left( \frac{m\pi}{2} \right) \sin^2 \left( \frac{n\pi}{2} \right) = \begin{cases} 0 & \text{for even } n \text{ or } m \\ \frac{4\alpha^2}{a^2} & \text{else.} \end{cases}$$

Since $E_n^0 - E_m^0 = \frac{\pi^2 \hbar^2}{2ma^2}(n^2 - m^2)$ we obtain:

$$E_n^2 = \frac{4\alpha^2}{a^2} \frac{2ma^2}{\pi^2 \hbar^2} \sum_{n \neq m, n=\text{odd}} \frac{1}{n^2 - m^2} = \frac{8m\alpha^2}{\pi^2 \hbar^2}, \quad -\frac{1}{4m^2} = -2m \left( \frac{\alpha}{\pi \hbar n} \right)^2$$  \hspace{1cm} (19)

where we have looked up the sum in a table. Note that $m$ outside the sum is the mass, not the summation index in the sum.

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3Revisit problem 1 where we computed $\langle \psi_0^m | H' | \psi_0^n \rangle$. 

5
b)

Q. Calculate the second-order correction to the ground state energy \( E_{20} \) for the potential in problem 6.2. Check that your result is consistent with the exact result obtained in problem 6.2 a) (eq.(9) in these solutions!).

Sol:
The second order correction to the ground state is:

\[
E_{20} = \sum_{m \neq 0} \frac{|\langle \psi_0^m | H' | \psi_0^0 \rangle|^2}{E_0^0 - E_m^0}
\]

and we are asked to consider the potential in problem 6.2. There we saw that the perturbation was:

\[
H' = \frac{1}{2} \epsilon k x^2
\]

and we exploited the ladder operators\(^4\)

\[
x^2 = \frac{\hbar}{2 \tilde{m} \omega} \left[ a_+^2 + a_+ a_- + a_- a_+ + a_-^2 \right] \tag{20}
\]

\[
a_+ \psi_n = \sqrt{n + 1} \psi_{n+1}, \quad a_- \psi_n = \sqrt{n} \psi_{n-1}. \tag{21}
\]

Now we have all the tools for solving the problem. Start by finding \( \langle \psi_0^m | H' | \psi_0^n \rangle \):

\[
\langle \psi_0^m | H' | \psi_0^n \rangle = \frac{1}{2} \epsilon k \frac{\hbar}{2 \tilde{m} \omega} \left[ \sqrt{n + 1} \sqrt{n + 2} \langle \psi_0^m | a_+^2 \psi_0^n \rangle + \sqrt{n} \sqrt{n + 1} \langle \psi_0^m | a_+ a_- | \psi_0^n \rangle + \sqrt{n} \sqrt{n - 1} \langle \psi_0^m | a_- a_+ | \psi_0^n \rangle + \langle \psi_0^m | a_-^2 | \psi_0^n \rangle \right]
\]

which gives:

\[
\langle \psi_0^m | H' | \psi_0^n \rangle = \frac{1}{2} \epsilon k \frac{\hbar}{2 \tilde{m} \omega} \left[ \sqrt{n + 1} \sqrt{n + 2} \langle \psi_0^m | \psi_0^n \rangle + \sqrt{n} \sqrt{n + 1} \langle \psi_0^m | \psi_0^n \rangle + \sqrt{n} \sqrt{n - 1} \langle \psi_0^m | \psi_0^n \rangle + \langle \psi_0^m | \psi_0^n \rangle \right]
\]

\(
(If \ you \ couldn't \ follow \ - \ revisit \ page \ 4 \ in \ this \ chapter \ of \ solutions \ for \ details.)
\)

Now, before we start computing \( |\langle \psi_0^m | H' | \psi_0^n \rangle|^2 \) we pause a moment and think. If we just square the expression above we will obtain 16 terms - lets first find out if we can skip some of them by thinking about their structure.

The 16 terms mentioned above will all contain the product of two (Kronecker) delta functions. If you now consider the product of two such that are not equal, say \( \delta_{m,n} \cdot \delta_{m,n+2} \) this has to be 0. For fun, try to prove this - it is a one line argument that is provided in the footnote-section on the next page.

\(^4\)Note that the mass is denoted \( \tilde{m} \) to avoid confusion with the index \( m \).
Since we don’t need to consider terms containing products of two distinct delta functions we obtain:

\[
|\langle \psi_0^m | H' | \psi_0^n \rangle|^2 = \epsilon^2 \frac{k^2 \hbar^2}{16 \tilde{m}^2 \omega^2} \left[(n+1)(n+2) (\delta_{m,n+2})^2 + n^2 (\delta_{m,n})^2 + (n+1) (\delta_{m,n})^2 + n(n-1) (\delta_{m,n-2})^2 \right].
\]

Now we can calculate \(E_0^2\):

\[
E_0^2 = \frac{\epsilon^2 k^2 \hbar^2}{16 \tilde{m}^2 \omega^2} \sum_{m \neq 0} \frac{1}{E_0^m - E_m^0} \left[(0 + 1)(0 + 2) (\delta_{m,0+2})^2 + 0(0 - 1) (\delta_{m,0+2})^2 \right]
\]

one of the delta functions collapses the sum:

\[
E_0^2 = \frac{\epsilon^2 k^2 \hbar^2}{16 \tilde{m}^2 \omega^2} \frac{2 \delta_{m,2}}{E_0^0 - E_2^0} = \frac{\epsilon^2 k^2 \hbar^2}{8 \tilde{m}^2 \omega^2} \frac{1}{E_0^0 - E_2^0}
\]

while the other one can be thrown away since it does nothing - there are no more indices \(m\) to force to the value 2.

Now we use:

\[
E_0^0 - E_2^0 = (0 + \frac{1}{2}) \hbar \omega - (2 + \frac{1}{2}) \hbar \omega = -2 \hbar \omega \quad \text{and} \quad k^2 = \tilde{m}^2 \omega^4
\]

to obtain:

\[
E_0^2 = \frac{\epsilon^2 \tilde{m}^2 \omega^4 \hbar^2}{8 \tilde{m}^2 \omega^2} \cdot \frac{1}{-2(2 \hbar \omega)} = \frac{\epsilon^2 \hbar \omega}{16}
\]

Note that the both the first order correction (eq.(17)) and second order correction (eq.(24)) are in agreement with the exact result obtained in eq.(9)!

Finally, here is the footnote for why the product of two distinct delta functions must be zero.\(^5\)

---

\(^5\)Consider \(\delta_{m,n+2} \cdot \delta_{m,n}\). The first delta function sets \(m = n + 2\) while the second sets \(m = n\). Combining these would mean \(n + 2 = n\) which has no solutions.
6.7

Q. Consider a particle of mass \( m \) that is free to move in a one-dimensional region of length \( L \) that closes on itself. An example of this would be problem 2.46 in the text book, where a bead slides frictionlessly on a circular wire.

a) Q. Show that the stationary states can be written in the form:

\[
\psi_n(x) = \frac{1}{\sqrt{L}} e^{\pm in\pi/L}, \quad (-L/2, < x < L/2)
\]

(25)

where \( n = 0, \pm 1, \pm 2, \ldots \) and the energies are given by:

\[
E_n = \frac{2m}{\hbar^2} \left( \frac{n\pi}{L} \right)^2.
\]

(26)

Notice that the spectrum is doubly degenerate for all \( n \) but \( n=0 \).

Sol:
The stationary states are the eigenstates of \( \hat{H} \) and to find these we solve the eigenvalue equation:

\[
\hat{H}\psi = E\psi.
\]

(27)

What is our \( \hat{H} \)? Recall that it normally has the form \( \hat{H} = T + V \), where \( T \) is the kinetic energy and \( V \) the potential.

In this particular case, the particle is moving freely so the potential is zero. Therefore, the Hamiltonian only contains the usual kinetic part:

\[
\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}.
\]

(28)

The eigenvalue equation to solve is thus\(^6\)

\[
\hat{H}\psi(x) = E\psi(x)
\]

\[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E\psi(x)
\]

which has solutions of the form:

\[
\psi(x) = Ce^{\pm ikx}
\]

(29)

with \( k = \sqrt{2mE/\hbar^2} \). These eigenfunctions are not yet fully determined - to do this we must know the values of \( k \) and \( C \). Here \( k \) is connected to the eigenvalues \( E \) and \( C \) is the normalization constant. We start by finding \( C \) from the condition:

\[
\langle \psi(x)|\psi(x) \rangle = 1
\]

(30)

---

\(^6\)You may have noticed that we went from \( \hat{H}\psi = E\psi \) in eq.(27) to \( \hat{H}\psi(x) = E\psi(x) \) and you might wonder why. It is not because \( |\psi\rangle = \psi(x) \), this is never the case! The reason is that in eq.(27), we did not specify in what basis \( \hat{H} \) was expressed. As soon as we used the position basis \( (x) \) the whole equation (27) was transformed into that basis.
which gives:

\[
\int_{-L/2}^{L/2} (e^{ikx})^* Ce^{ikx} \, dx = |C|^2 \int_{-L/2}^{L/2} 1 \, dx \quad \Rightarrow \quad C = \frac{1}{\sqrt{L}} \tag{31}
\]

Now we find the allowed values for \( k \) (and thus also for \( E \)). We do this by applying the boundary condition which in this case is that the functions are periodic\(^7\):

\[
\psi(-\frac{L}{2}) = \psi(\frac{L}{2}) \quad \Rightarrow \quad Ce^{-ik\frac{L}{2}} = Ce^{ik\frac{L}{2}} \quad \Rightarrow \quad 1 = e^{ikL}
\]

Recall that \( 1 = e^{i2\pi n} \) for all integers \( n \). Inserting this into the box gives:

\[
e^{ikL} = e^{i2\pi n} \, \forall n \in \mathbb{Z} \quad \Rightarrow \quad kL = 2n\pi \, \forall n \in \mathbb{Z}.
\]

Combining this result with \( k = \sqrt{2mE/\hbar^2} \) gives:

\[
k = \frac{2n\pi}{L} \quad \Rightarrow \quad \sqrt{\frac{2mE}{\hbar^2}} = \frac{2n\pi}{L} \quad \Rightarrow \quad E_n = \frac{2m}{\hbar^2} \left( \frac{2n\pi}{L} \right)^2 \forall n \in \mathbb{Z}. \tag{32}
\]

Thus:

\[
\psi_n(x) = \frac{1}{\sqrt{L}} e^{i\frac{2n\pi x}{L}} \, \forall n \in \mathbb{Z} \tag{33}
\]

\[
E_n = \frac{2m}{\hbar^2} \left( \frac{2n\pi}{L} \right)^2 \forall n \in \mathbb{Z}. \tag{34}
\]

\(^7\)since the problem statement says that the region closes on itself
Q. Now suppose we introduce the perturbation:

\[ H' = -V_0 e^{-x^2/a^2} \]  \hspace{1cm} (35)

where \( a << L \).

Find the first-order correction to \( E_n \) using eq.(6.27) in the text book. Hint: to evaluate the integral, exploit the fact that \( a << L \) to extend the limits from \( \pm L/2 \) to \( \pm \infty \).

Sol:

The first-order correction for degenerate perturbation theory is given by eq.(6.27) in the text book:

\[ E_1^{\pm} = \frac{1}{2} \left[ W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2} \right] \]  \hspace{1cm} (36)

where:

\[ W_{ab} \equiv \langle \psi_0^a | H' | \psi_0^b \rangle \]  \hspace{1cm} (37)

and the indices \( a, b \) denote that indices for the degenerate energy levels. In this example the energy levels are degenerate for \( \pm n \), so \( a = n, \ b = -n \).

Now we calculate \( W_{nn} \):

\[ W_{nn} = \langle \psi_n^0 | H' | \psi_n^0 \rangle = \int \frac{L}{2} \frac{1}{\sqrt{L}} e^{-i \frac{2\pi n x}{L}} \left[ -V_0 e^{-x^2/a^2} \right] \frac{1}{\sqrt{L}} e^{i \frac{2\pi n x}{L}} dx = -\frac{V_0}{L} \int \frac{L}{2} e^{-x^2/a^2} dx \]

If we now use the hint \( a << L \) we obtain an integral that we can look up:

\[ W_{nn} = -\frac{V_0}{L} \int \frac{L}{2} e^{-x^2/a^2} dx \approx -\frac{V_0}{L} \int_{-\infty}^{\infty} e^{-x^2/a^2} dx = -\frac{V_0}{L} \frac{\sqrt{\pi}}{a} \]  \hspace{1cm} (38)

Looking at eq.(36) we see that we also have to calculate \( W_{n,-n} \):

\[ \langle \psi_n^0 | H' | \psi_{-n}^0 \rangle = -\frac{V_0}{L} \int_{-L/2}^{L/2} e^{-i \frac{2\pi n x}{L}} e^{-x^2/a^2} e^{-i \frac{2\pi n x}{L}} dx = -\frac{V_0}{L} \int_{-L/2}^{L/2} e^{-\frac{x^2}{a^2} - i \frac{2\pi n x}{L}} dx \]

Once again, we use the approximation given in the hint:

\[ \langle \psi_n^0 | H' | \psi_{-n}^0 \rangle \approx -\frac{V_0}{L} \int_{-\infty}^{\infty} e^{-\frac{x^2}{a^2} - i \frac{2\pi n x}{L}} dx \]

---

\(^8\) Why can we do this? If you don’t see it, think of the integral as a sum. What happens to \( e^{-x^2/a^2} \) for large values of \( x \) and small values of \( a \)?
This integral is a bit complicated. If the QM course you are following does not require you to have taken a mathematics course in complex analysis you are most likely getting the following result on a sheet of formulae:

\[
\int_{-\infty}^{\infty} e^{-\frac{x^2}{\alpha^2} - i \frac{4n\pi x}{L}} dx = e^{-(\frac{2n\pi a}{L})^2} a \sqrt{\pi}
\]  
(39)

using this we obtain:

\[
W_{n_0,n} \approx -V_0 e^{-(\frac{2n\pi a}{L})^2} a \sqrt{\pi}
\]

which together with eq.(38) inserted into eq.(36) gives:

\[
E_{1\pm} = -V_0 e^{-(\frac{2n\pi a}{L})^2} a \sqrt{\pi} \left( 1 \mp e^{-(\frac{2n\pi a}{L})^2} \right)
\]

(41)

For the interested reader we provide some details about eq.(39). Remember that these are most likely overkill if you are taking a QM course using this text book so skip them if you are not interested.

Completing the square\(^9\) gives:

\[
\int_{-\infty}^{\infty} e^{-\frac{x^2}{\alpha^2} - i \frac{4n\pi x}{L}} dx = \int_{-\infty}^{\infty} e^{-\left(\frac{x}{\alpha} + i \frac{2n\pi}{L}\right)^2} e^{-(\frac{2n\pi a}{L})^2} \int_{-\infty}^{\infty} e^{-\left(\frac{y}{\alpha} + i \frac{2n\pi}{L}\right)^2} dy.
\]

Make the variable substitution:

\[
x = \frac{y}{\alpha} + i \frac{2n\pi}{L}, \quad dx = \alpha dy, \quad -\infty < y < \infty
\]

which gives:

\[
\int_{-\infty}^{\infty} e^{-\left(\frac{y}{\alpha} + i \frac{2n\pi}{L}\right)^2} dy = \alpha \int_{-\infty}^{\infty} e^{-y^2} dy.
\]

(42)

The right hand side is a very famous integral that is tabulated in most places. However, the limits are now complex which might be a first sight for most of you. Using something called the Cauchy residue theorem\(^10\) one sees that this integral is the same as if it had been computed on the real line. Thus, in this case, you can just ignore the imaginary parts in the integration limits to obtain:

\[
\int_{-\infty}^{\infty} e^{-\left(\frac{y}{\alpha} + i \frac{2n\pi}{L}\right)^2} dy = a \int_{-\infty}^{\infty} e^{-y^2} dy = a \sqrt{\pi}.
\]

(43)

\(^9\)In Swedish: kvadratkomplettering.

\(^10\)In the beautiful theory of complex analysis you learn how to overcome the many limits in real-valued mathematical analysis. You also explain a lot of the weird trigonometric substitutions suggested for solving real valued integrals.
Q. What are the "good" linear combinations of $\psi_n$ and $\psi_{-n}$ for this problem? Show that with these states you get the first-order correction using eq.(6.9) in the text book. (Note: this is the first order correction for nondegenerate perturbation theory.)

Sol:
Let us start by clarify the goals of this problem:
1) Find the "good" linear combinations of the degenerate states $\psi_n$ and $\psi_{-n}$.
2) Using these good states, verify that the first order nondegenerate energy correction gives the same answer as eq.(41).

In the case of a two-fold degeneracy the "good" states must be of the form:

$$\psi = \alpha \psi_0^a + \beta \psi_0^b$$ (44)

Eq.(6.22) in the text book gives:

$$\alpha W_{aa} + \beta W_{ab} = \alpha E^1 \implies \beta = \alpha \frac{E^1 - W_{aa}}{W_{ab}}$$

so in our case we obtain:

$$\beta_+ = \alpha_+ \frac{E^1_+ - W_{aa}}{W_{ab}} \quad \beta_- = \alpha_- \frac{E^1_- - W_{aa}}{W_{ab}}$$ (45)

Recall that we computed $W_{aa}, W_{ab}, E^1_\pm$ in the previous problem ($a=n, b=-n$). We will now use information about these to obtain the coefficients in eq.(45).

From eq.(36) and eq.(38) we see that:

$$E^1_\pm = W_{nn} \mp |W_{n,-n}|$$ (46)

which inserted into eq.(45) gives:

$$\beta_+ = \frac{-|W_{n,-n}|}{W_{n,n}} \alpha_+ \quad \beta_- = \frac{|W_{n,-n}|}{W_{n,n}} \alpha_-$$

Using the result in eq.(40) we now obtain:

$$\beta_+ = \alpha_+ \quad \beta_- = -\alpha_-.$$ (47)

Finally, we are now able to give the "good" linear combinations:

$$\psi_+ = \alpha_+ \psi_n + \beta_+ \psi_{-n} = \alpha_+ \psi_n - \alpha_+ \psi_{-n} = \frac{\alpha_-}{\sqrt{L}} \left( e^{i \frac{2\pi n x}{L}} - e^{-i \frac{2\pi n x}{L}} \right) = \frac{2 \alpha_+}{\sqrt{L}} \sin \left( \frac{2\pi n x}{L} \right)$$

$$\psi_- = \alpha_- \psi_n + \beta_- \psi_{-n} = \alpha_- \psi_n + \alpha_- \psi_{-n} = \frac{\alpha_-}{\sqrt{L}} \left( e^{i \frac{2\pi n x}{L}} + e^{-i \frac{2\pi n x}{L}} \right) = \frac{2 \alpha_-}{\sqrt{L}} \cos \left( \frac{2\pi n x}{L} \right)$$
To determine $\alpha_{\pm}$ you can either compute the integrals or just note that since we added two orthonormal functions to create $\psi_{\pm}$ we must have $\alpha_{+} = \alpha_{-} = \frac{1}{\sqrt{2}}$.

**Now we will attack the second part of the problem:** calculate the first order energy corrections $E_{\pm}^{1}$ for nondegenerate states by using the good states that we have just found:

$$\psi_{+} = \sqrt{\frac{2}{L}} \sin \left( \frac{2\pi n}{L} x \right) \quad \psi_{-} = \sqrt{\frac{2}{L}} \cos \left( \frac{2\pi n}{L} x \right)$$ (48)

We will in this solution do $E_{+}^{1} = \langle \psi_{+} | H' | \psi_{+} \rangle$ and leave the other case as an exercise.

$$E_{+}^{1} = \langle \psi_{+} | H' | \psi_{+} \rangle = \langle \psi_{+} | - V_0 e^{-x^2/a^2} | \psi_{+} \rangle = - \frac{2}{L} V_0 \int_{-L/2}^{L/2} e^{-\frac{x^2}{a^2}} \sin^2 \left( \frac{2\pi nx}{L} \right) dx$$ (49)

using the hint from the previous problems:

$$\int_{-L/2}^{L/2} e^{-\frac{x^2}{a^2}} \sin^2 \left( \frac{2\pi nx}{L} \right) dx \approx \int_{-\infty}^{\infty} e^{-\frac{x^2}{a^2}} \sin^2 \left( \frac{2\pi nx}{L} \right) dx.$$ (50)

Using Euler’s formula we obtain:

$$\int_{-\infty}^{\infty} e^{-\frac{x^2}{a^2}} \sin^2 \left( \frac{2\pi nx}{L} \right) dx = \int_{-\infty}^{\infty} e^{-\frac{x^2}{a^2}} \left( e^{\frac{4\pi nx}{L}} + e^{-\frac{4\pi nx}{L}} - 2 \right) dx$$

$$= \frac{1}{4} \int_{-\infty}^{\infty} e^{-x^2/a^2} e^{4\pi nx/L} dx - \frac{1}{4} \int_{-\infty}^{\infty} e^{-x^2/a^2} e^{-4\pi nx/L} dx + \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2/a^2} dx. \quad (51)$$

Like in the previous problem, the first two integrals are mean. Therefore we just give the results:

$$\int_{-\infty}^{\infty} e^{-x^2/a^2} e^{4\pi nx/L} dx = \int_{-\infty}^{\infty} e^{-x^2/a^2} e^{-4\pi nx/L} dx = e^{-\left( \frac{2\pi na}{L} \right)^2} a \sqrt{\pi} \quad (52)$$

So combining eq.(52), eq.(51) and eq.(49) gives:

$$E_{+}^{1} = - \frac{V_0}{L} a \sqrt{\pi} \left[ 1 - e^{-\left( \frac{2\pi na}{L} \right)^2} \right]$$ (53)

which is in agreement with eq.(41), the result obtained using degenerate perturbation theory. Now you should verify that you have understood the solution by redoing the steps for $E_{-}^{1}$.

\[11\text{As a fun exercise, prove the second step. You don’t need any complex analysis for that.}\]
6.9

Q. Consider a quantum system with just three linearly independent states. Suppose the Hamiltonian in matrix form is:

\[ H = V_0 \begin{pmatrix} 1 - \epsilon & 0 & 0 \\ 0 & 1 + \epsilon & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix} \]  

(54)

where \( V_0 \) is a constant and \( \epsilon \ll 1 \).

a)

Q. Write down the eigenvectors and eigenvalues of the unperturbed Hamiltonian (\( \epsilon = 0 \)).

Sol:

This is very straightforward. If \( \epsilon = 0 \) then:

\[ H_0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \]  

(55)

and we immediately see that the eigenvectors are:

\[ |\alpha_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\alpha_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |\alpha_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \]  

(56)

with the three eigenvalues:

\[ \lambda_1 = V_0, \quad \lambda_2 = V_0, \quad \lambda_3 = 2V_0 \]  

(57)

b)

Q. Solve for the exact eigenvalues of \( H \). Expand each of them as a power series in \( \epsilon \) up to second order.

Sol:

This is something that we have done a lot. Start by setting up the eigenvalue matrix equation:

\[ H|\alpha\rangle = \lambda|\alpha\rangle \]

\[ V_0 \begin{pmatrix} 1 - \epsilon & 0 & 0 \\ 0 & 1 + \epsilon & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \\ c \end{pmatrix} \]

\[ \implies \begin{vmatrix} V_0(1 - \epsilon) - \lambda & 0 & 0 \\ 0 & V_0 - \lambda & V_0\epsilon \\ 0 & V_0\epsilon & 2V_0 - \lambda \end{vmatrix} = 0 \]
\[
(V_0(1 - \epsilon) - \lambda)(V_0 - \lambda)(2V_0 - \lambda) - V_0 \epsilon \cdot V_0 \epsilon \cdot (V_0(1 - \epsilon) - \lambda) = 0
\]

\[
(V_0(1 - \epsilon) - \lambda) [(V_0 - \lambda)(2V_0 - \lambda) - V_0 \epsilon \cdot V_0 \epsilon] = 0
\]

\[
(V_0(1 - \epsilon) - \lambda) [\lambda^2 - 3V_0 \lambda + V_0^2 (2 - \epsilon^2)] = 0
\]

which has the solutions:

\[
(V_0(1 - \epsilon) - \lambda) = 0 \iff \lambda_1 = V_0(1 - \epsilon)
\]

\[
\lambda^2 - 3V_0 \lambda + V_0^2 (2 - \epsilon^2) \iff \lambda_2 = \frac{V_0}{2} \left(3 - \sqrt{1 + 4 \epsilon^2}\right) \quad \lambda_3 = \frac{V_0}{2} \left(3 + \sqrt{1 + 4 \epsilon^2}\right)
\]

expanding \(\sqrt{1 + 4 \epsilon^2} \approx 1 + 2 \epsilon^2 + \ldots\) gives:

\[
\lambda_1 \approx V_0 - \epsilon V_0
\]

\[
\lambda_2 \approx V_0 - \epsilon^2 V_0
\]

\[
\lambda_3 \approx 2V_0 + \epsilon^2 V_0
\]

\[N.B: \text{ we chose } \lambda_2 = \frac{V_0}{2} \left(3 - \sqrt{1 + 4 \epsilon^2}\right) \text{ out of convenience. We could have chosen the other square root instead if we wanted to.}\]

c)

Q. Use first- and second-order nondegenerate perturbation theory to find the approximate eigenvalue for the state that grows out of the nondegenerate eigenvector of \(H^0\). Compare this to the exact value obtained in (a).

Sol:

For nondegenerate perturbation theory we get the first order correction from:

\[
E_n^1 = \langle \alpha_n^0 | H' | \alpha_n^0 \rangle
\]

and since our perturbation (on matrix form) is:

\[
H' = \epsilon V_0 \begin{pmatrix}
-1 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0
\end{pmatrix}
\]

and the state that is nondegenerate is the one with the unperturbed eigenvalue \(2V_0\) we find:

\[
E_n^1 = \langle \alpha_3^0 | H' | \alpha_3^0 \rangle = (0 \quad 0 \quad 1) \epsilon V_0 \begin{pmatrix}
-1 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0
\end{pmatrix} \begin{pmatrix}
0 \\
0 \\
1
\end{pmatrix} = 0
\]

15
(which means that there is no first-order energy correction due to the perturbation).

The second-order correction is given by:

\[
E_3^2 = \sum_{m \neq 3} \frac{|\langle \alpha_0^m | H' | \alpha_0^3 \rangle|^2}{E_3^0 - E_m^0} = \frac{|\langle \alpha_0^0 | H' | \alpha_0^0 \rangle|^2}{E_3^0 - E_1^0} + \frac{|\langle \alpha_0^0 | H' | \alpha_0^0 \rangle|^2}{E_3^0 - E_2^0}
\]

(64)

and computing the inner products:

\[
\langle \alpha_0^0 | H' | \alpha_0^3 \rangle = (1 \ 0 \ 0) \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0
\]

(65)

\[
\langle \alpha_0^0 | H' | \alpha_0^3 \rangle = (0 \ 1 \ 0) \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \epsilon V_0
\]

(66)

gives:

\[
E_3^2 = \frac{|\langle \alpha_0^0 | H' | \alpha_0^0 \rangle|^2}{E_3^0 - E_2^0} = \frac{\epsilon^2 V_0^2}{2V_0 - V_0} = \epsilon^2 V_0
\]

(67)

which is the same as the result you obtained in (a).
Q. Use degenerate perturbation theory to find the first-order correction to the two initially degenerate eigenvalues. Compare to the exact results.

Sol:

First order degenerate perturbation theory gives the energy correction:

$$E_{\pm}^1 = \frac{1}{2} \left[ W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2} \right]$$  \hspace{1cm} (68)

with $W_{ab} \equiv \langle \alpha_0^a | H' | \alpha_0^b \rangle$.

Our degenerate states are $a=1$ and $b=2$ so we obtain:

$$W_{11} = (1 \ 0 \ 0) \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = -\epsilon V_0$$

$$W_{12} = (1 \ 0 \ 0) \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

$$W_{22} = (0 \ 1 \ 0) \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

Insert these results into eq.(68) to obtain:

$$E_{\pm}^1 = \frac{1}{2} \left[ -\epsilon V_0 \pm \sqrt{(-\epsilon V_0 - 0)^2 + 0} \right] = \begin{cases} 0 \text{ for } E_{+}^1 \\ -\epsilon V_0 \text{ for } E_{-}^1 \end{cases}$$  \hspace{1cm} (69)

Is this consistent with the results in (b)? Yes, because there we found:

$$E_{1}^1 = V_0 \lambda - \epsilon V_0$$  \hspace{1cm} (70)

$$E_{2}^1 = V_0 \lambda - \epsilon^2 V_0$$  \hspace{1cm} (71)

and in this problem we found that one state gets forced down by $-\epsilon V_0$ while the other state is unaffected in first order of $\epsilon$. 

6.32

Q. Suppose the Hamiltonian $\hat{H}$ for a particular quantum system is a function of some parameter $\lambda$; let $E_n(\lambda)$ and $\psi_n(\lambda)$ be the eigenvalues and eigenfunctions of $H(\lambda)$. The Feynman-Hellmann theorem states that

$$\frac{\partial E_n}{\partial \lambda} = \left\langle \psi_n \left| \frac{\partial H}{\partial \lambda} \right| \psi_n \right\rangle$$

(72)

assuming either that $E_n$ is nondegenerate or if degenerate that the $\psi_n$’s are the “good” linear combinations of the degenerate eigenfunctions.

a)


Sol:

There are at least two ways to prove this theorem. We first present the suggested way by the problem statement and then the original way Feynman did it as an alternative.

Method 1

Since $H$ is a function of $\lambda$ everything changes according to $\lambda$. To organize our thoughts, let us first define a fixed point $\lambda = \lambda_0$ and then observe a change from this fixed point:

$$H(\lambda_0 + d\lambda) = H(\lambda_0) + V(\lambda_0 + d\lambda) = H_0 + H'(\lambda_0 + d\lambda)$$

(73)

the purpose of this is to reconnect with our notion of perturbation. Whatever changes our Hamiltonian is due to the last term, which is the perturbation.

We can identify this perturbation in the spirit of a true physicist by using a power series expansion of the new Hamiltonian:

$$H(\lambda_0 + d\lambda) = H_0 + \frac{\partial H(\lambda_0)}{\partial \lambda} d\lambda + O(d\lambda^2) + \ldots$$

(74)

everything after $H_0$ in eq.(74) would thus be our perturbation. We shall however soon see that we only need to consider the first term.

Now consider the left hand side of eq.(72). (Our aim is to use valid manipulations that end up with the right hand side of eq.(72)).

For our fixed point $\lambda = \lambda_0$ the left hand side can be written as:

$$\frac{\partial E_n(\lambda_0)}{\partial \lambda} = \lim_{d\lambda \to 0} \frac{E_n(\lambda_0 + d\lambda) - E_n(\lambda_0)}{d\lambda} = \lim_{d\lambda \to 0} \frac{E_n^1(\lambda_0 + d\lambda)}{d\lambda}$$

(75)

where the last step is valid since $E_n(\lambda_0 + d\lambda) = E_n(\lambda_0) + E_n^1(\lambda_0 + d\lambda)$ for small enough $d\lambda$. 

18
According to eq.(6.9) in the text book (first order nondegenerate energy correction):

\[ E_n^1(\lambda_0 + d\lambda) = \langle \psi_n^0 | H'(\lambda_0 + d\lambda) | \psi_n^0 \rangle. \]  

(76)

so eq.(75) now becomes:

\[ \frac{\partial E_n(\lambda_0)}{\partial \lambda} = \lim_{d\lambda \to 0} \frac{\langle \psi_n^0 | H'(\lambda_0 + d\lambda) | \psi_n^0 \rangle}{d\lambda} = \langle \psi_n^0 | \lim_{d\lambda \to 0} \frac{H'(\lambda_0 + d\lambda)}{d\lambda} | \psi_n^0 \rangle \]  

(77)

where the last step is valid because \(d\lambda\) is just a scalar. Notice that it is reassuring that our result resembles eq.(72).

Proceeding now with the right hand side of eq.(77) we recall the power series expansion in eq.(74):

\[ H(\lambda_0 + d\lambda) = H_0 + \frac{\partial H(\lambda_0)}{\partial \lambda} d\lambda + O(d\lambda^2) + \ldots = H_0 + H'(\lambda_0 + d\lambda) \]

From this we see that:

\[ \lim_{d\lambda \to 0} \frac{H'(\lambda_0 + d\lambda)}{d\lambda} = \frac{\partial H(\lambda_0)}{\partial \lambda} \]

(78)

which gives us a new form of eq.(77):

\[ \frac{\partial E_n(\lambda_0)}{\partial \lambda} = \langle \psi_n^0 | \frac{\partial H(\lambda_0)}{\partial \lambda} | \psi_n^0 \rangle \]  

(79)

Now we are almost done. Recall that \(\psi_n^0\) are the unperturbed eigenfunctions and can be written as \(\psi_n^0 = \psi_n(\lambda_0)\). So eq.(79) has a more general form:

\[ \frac{\partial E_n(\lambda_0)}{\partial \lambda} = \langle \psi_n(\lambda_0) | \frac{\partial H(\lambda_0)}{\partial \lambda} | \psi_n(\lambda_0) \rangle \]  

(80)

Finally, notice that eq.(80) was obtained by taking a small step \(d\lambda\) from the starting value \(\lambda_0\). Obviously, we could take another step \(d\lambda\) again, redoing all the calculations on the last two pages, to obtain:

\[ \frac{\partial E_n(\lambda_0 + d\lambda)}{\partial \lambda} = \langle \psi_n(\lambda_0 + d\lambda) | \frac{\partial H(\lambda_0 + d\lambda)}{\partial \lambda} | \psi_n(\lambda_0 + d\lambda) \rangle. \]  

(81)

The last line of argument was our final piece to conclude the proof of:

\[ \frac{\partial E_n(\lambda)}{\partial \lambda} = \langle \psi_n(\lambda) | \frac{\partial H(\lambda)}{\partial \lambda} | \psi_n(\lambda) \rangle \]  

(82)
Method (2)
In this alternative method we do not use perturbation theory but work with the left hand side of eq.(72) directly:

\[
\frac{\partial E_n}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left[ \langle \psi_n | H | \psi_n \rangle \right]
\]

\[
= \left\langle \left\langle \frac{\partial \psi_n}{\partial \lambda} \right\vert H \right\vert \psi_n \rangle + \left\langle \psi_n \left\langle \frac{\partial H}{\partial \lambda} \right\vert \psi_n \rangle + \left\langle \psi_n \left\langle \frac{\partial H}{\partial \lambda} \right\vert \psi_n \rangle \right. \\
\]

\[
= \left\langle \frac{\partial \psi_n}{\partial \lambda} \right\vert E_n \left\vert \psi_n \rangle + \left\langle \psi_n \left\langle \frac{\partial H}{\partial \lambda} \right\vert \psi_n \rangle + \left\langle \psi_n \left\langle \frac{\partial H}{\partial \lambda} \right\vert \psi_n \rangle \right. \\
\]

\[
= E_n \left\langle \frac{\partial \psi_n}{\partial \lambda} \right\vert \psi_n \rangle + \left\langle \psi_n \left\langle \frac{\partial H}{\partial \lambda} \right\vert \psi_n \rangle + \left\langle \psi_n \left\langle \frac{\partial H}{\partial \lambda} \right\vert \psi_n \rangle \right. \\
\]

but remember now that the energies are real, so \( E_n^* = E_n \). Thus:

\[
\frac{\partial E_n}{\partial \lambda} = \left\langle \psi_n \left\langle \frac{\partial H}{\partial \lambda} \right\vert \psi_n \rangle + E_n \frac{\partial}{\partial \lambda} [\langle \psi_n | \psi_n \rangle] \right. \\
\]

(83)

where we have used that \( \langle \psi_n | \psi_n \rangle = 1 \), so the last term is 0.
b)  

Q. Apply the theorem to the one-dimensional harmonic oscillator, (i) using \( \lambda = \omega \) (which yields a formula for \( \langle V \rangle \)), (ii) using \( \lambda = \hbar \) (which yields a formula for \( \langle T \rangle \)) and (iii) using \( \lambda = m \) (which yields a relation between \( \langle V \rangle \) and \( \langle T \rangle \)). Compare your answers to problem 2.12 and the Virial theorem predictions.

Sol:

Here we are going to use the formula we proved in the previous problem:

\[
\frac{\partial E_n}{\partial \lambda} = \langle \psi_n \mid \frac{\partial H}{\partial \lambda} \mid \psi_n \rangle
\]

for the harmonic oscillator. The Hamiltonian and the energies are given by:

\[
H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \quad \quad E_n = \hbar \omega \left( n + \frac{1}{2} \right) \tag{84}
\]

(i) Using this for \( \lambda = \omega \) we get:

\[
\frac{\partial E_n}{\partial \omega} = \langle \psi_n \mid \frac{\partial H}{\partial \omega} \mid \psi_n \rangle = \langle \psi_n \mid m \omega^2 x^2 \mid \psi_n \rangle = \langle \psi_n \mid 2V \omega \mid \psi_n \rangle
\]

From the energies we then see:

\[
\frac{\partial E_n}{\partial \omega} = \hbar \left( n + \frac{1}{2} \right) = \frac{E_n}{\omega}
\]

and thus:

\[
E_n = 2 \langle V \rangle \tag{85}
\]

which is familiar from problems 2.12 and 3.31.

(ii) Using \( \lambda = \hbar \) instead we now get:

\[
\frac{\partial E_n}{\partial \hbar} = \langle \psi_n \mid \frac{\partial H}{\partial \hbar} \mid \psi_n \rangle = \langle \psi_n \mid -\frac{\hbar}{m} \frac{d^2}{dx^2} \mid \psi_n \rangle = \langle \psi_n \mid \frac{2}{\hbar} T \mid \psi_n \rangle = \frac{2}{\hbar} \langle T \rangle. \tag{86}
\]

From the expression for the energies you get (check this):

\[
\frac{\partial E_n}{\partial \hbar} = \frac{E_n}{\hbar}
\]

so eq.(77) gives:

\[
E_n = 2 \langle T \rangle. \tag{87}
\]

Now you can do the third exercise (iii) to verify what you can get from (i) and (ii): \( \langle V \rangle = \langle T \rangle \).