

Homework 7

TA: Renée Goodman, Due: Tuesday, February 27th, 2024, 11:59 PM

March 8, 2024

1. (5 Points) **Townsend 11.1** Consider a perturbation $\hat{H}_1 = b\hat{x}^4$ to the simple harmonic oscillator Hamiltonian

$$\hat{H}_0 = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \quad (1)$$

This is an example of an anharmonic oscillator, one with a non-linear restoring force.

- (a) Show that the first-order shift in the energy is given by:

$$E_n^{(1)} = \frac{3\hbar^2 b}{4m^2\omega^2}(1 + 2n + n^2) \quad (2)$$

Solution: From Townsend Eq. 11.15 the first order energy shift is given by:

$$E_n^{(1)} = \langle \Psi_n^{(0)} | \hat{H}_1 | \Psi_n^{(0)} \rangle \quad (3)$$

Where \hat{H}_1 is the perturbation to the Hamiltonian, and $|\Psi_n^{(0)}\rangle$ are the unperturbed wave functions. For the simple harmonic oscillator we will use $|\Psi_n^{(0)}\rangle = |n\rangle$ and we will write the perturbation in terms of the raising and lowering operators a and a^\dagger . We therefore get the expression:

$$E_n^{(1)} = \langle n | b \left(\frac{\hbar}{2m\omega} \right)^2 (a + a^\dagger)^4 | n \rangle \quad (4)$$

Recalling that $[a, a^\dagger] = 1$, we can expand $(a + a^\dagger)^4$ into $(a + a^\dagger)^2 (a + a^\dagger)^2$ to get:

$$E_n^{(1)} = b \left(\frac{\hbar}{2m\omega} \right)^2 \langle n | [a^2 + aa^\dagger + a^\dagger a + a^{\dagger 2}] [a^2 + aa^\dagger + a^\dagger a + a^{\dagger 2}] | n \rangle \quad (5)$$

$$E_n^{(1)} = b \left(\frac{\hbar}{2m\omega} \right)^2 \langle n | [a^2 + 1 + 2a^\dagger a + a^{\dagger 2}] [a^2 + 1 + 2a^\dagger a + a^{\dagger 2}] | n \rangle \quad (6)$$

We can take the left part to act on $\langle n |$ and the right side to act on $|n\rangle$. Using the definitions of a and a^\dagger

$$a |n\rangle = \sqrt{n+1} |n+1\rangle; \quad a^\dagger |n\rangle = \sqrt{n} |n-1\rangle \quad (7)$$

we can determine how each term acts on $|n\rangle$:

$$a^2 |n\rangle = \sqrt{n+1}\sqrt{n+2} |n+2\rangle; \quad a^{\dagger 2} |n\rangle = \sqrt{n}\sqrt{n-1} |n-2\rangle \quad (8)$$

$$aa^\dagger |n\rangle = n |n\rangle; \quad a^\dagger a |n\rangle = (n+1) |n\rangle \quad (9)$$

Recall the states $|n\rangle$ form an orthonormal basis, therefore any cross-terms go to 0 and we get:

$$E_n^{(1)} = b \left(\frac{\hbar}{2m\omega} \right)^2 [(n+1)(n+2) + n(n-1) + 1 + 4n(n+1)] \quad (10)$$

$$E_n^{(1)} = 3b \left(\frac{\hbar}{2m\omega} \right)^2 [2n^2 + 2n + 1] \quad (11)$$

- (b) Argue that no matter how small b is, the perturbation expansion will break down for some sufficiently large n . What is the physical reason?

Solution: We see that $E_n^{(1)}$ is linear in b and quadratic in n . Therefore as n becomes large, we will no longer have $E_n^{(0)} \gg E_n^{(1)}$ regardless of b , which is necessary to use perturbation theory. The physical reasoning is that the particle will explore larger values of x , and the system no longer behaves like a quantum harmonic oscillator as the x^4 term will dominate the potential for large enough x .

2. (9 points) An infinite square well between $x = -a$ and $x = a$ is perturbed by a potential $V_1(x) = \lambda x/a$, where $\lambda \ll 1$. Show that to first order in λ , (a) the energy levels are unchanged, whereas (b) the ground state wave function is changed. Derive an expression for the ground state wave function $\psi(x)$ that includes the first order correction, evaluating all necessary integrals. Make a plot of $\psi(x)$ and compare with the original ground state wave function, explaining whether the difference makes sense physically.

Solution:

- (a) Using the definition of the energy:

$$E_n = E_0 + \lambda E_1 = E_0 + \langle \psi_n(x) | V_1(x) | \psi_n(x) \rangle \quad (12)$$

where $|\psi_n(x)\rangle$ are the unperturbed wave functions. To show that the energy levels are unchanged, we simply must show that $\langle \psi_n(x) | V_1(x) | \psi_n(x) \rangle = 0$:

$$\langle \psi_n(x) | V_1(x) | \psi_n(x) \rangle = \frac{\lambda}{a} \langle \psi_n(x) | x | \psi_n(x) \rangle = \frac{\lambda}{a} \langle x \rangle \quad (13)$$

Recall for an unperturbed infinite square well, $\langle x \rangle = 0$ for all n since $|\psi(x)|^2$ is symmetric about $x = 0$. Therefore $\langle \psi_n(x) | V_1(x) | \psi_n(x) \rangle = 0$ and the energy levels are unchanged.

- (b) From Townsend Eq. 11.23, the corrected wave function is given by

$$|\psi_n(x)\rangle = |\psi_n^{(0)}\rangle + \sum_{k \neq n} |\psi_k^{(0)}\rangle \frac{\langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} \quad (14)$$

For an infinite square well of length $2a$ the unperturbed wave function $\psi_n^{(0)}$ is given by

$$\psi_n^{(0)} = \begin{cases} \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a}\right), & n = \text{even} \\ \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a}\right), & n = \text{odd} \end{cases} \quad (15)$$

with energies

$$E_n^{(0)} = \frac{n^2 \hbar^2}{8ma^2} \quad (16)$$

We want the ground state correction, so here $n = 1$. Beginning with the $\langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle$ term (we only need to consider even $\psi_k^{(0)}(x)$ as when we compute this with odd $\psi_k^{(0)}(x)$ the integral will be 0):

$$\langle \psi_k^{(0)} | \hat{H}_1 | \psi_1^{(0)} \rangle = \frac{\lambda}{a^2} \int_{-a}^a dx \sin\left(\frac{k\pi x}{2a}\right) x \cos\left(\frac{\pi x}{2a}\right) \quad (17)$$

This integral can be evaluated to give:

$$\langle \psi_k^{(0)} | \hat{H}_1 | \psi_1^{(0)} \rangle = -\frac{16\lambda}{\pi^2} \left(\frac{k}{(1-k^2)^2} \right) \cos\left(\frac{k\pi x}{2a}\right) \sin\left(\frac{\pi x}{2a}\right) \Big|_{-a}^a \quad (18)$$

Evaluating at the endpoints.

$$\langle \psi_k^{(0)} | \hat{H}_1 | \psi_1^{(0)} \rangle = -\frac{16\lambda}{\pi^2} \left(\frac{k}{(1-k^2)^2} \right) \cos\left(\frac{\pi k}{2}\right) = -\frac{16\lambda}{\pi^2} \left(\frac{(-1)^{k/2}k}{(1-k^2)^2} \right) \quad (19)$$

for an integer k . Per Townsend 11.23, our corrected wave function then becomes for even k :

$$|\psi_1(x)\rangle = \sqrt{\frac{1}{a}} \cos\left(\frac{\pi x}{2a}\right) - \frac{16\lambda}{\pi^2} \left(\frac{8ma^2}{\hbar^2} \right) \sum_{k \neq 1} \frac{(-1)^{k/2}k}{(1-k^2)^3} \sin\left(\frac{k\pi x}{2a}\right) \quad (20)$$

The plot of the perturbed vs unperturbed wave function shows that the wavelength increases or decreases with the potential V_1 . See Appendix for the coding solution.

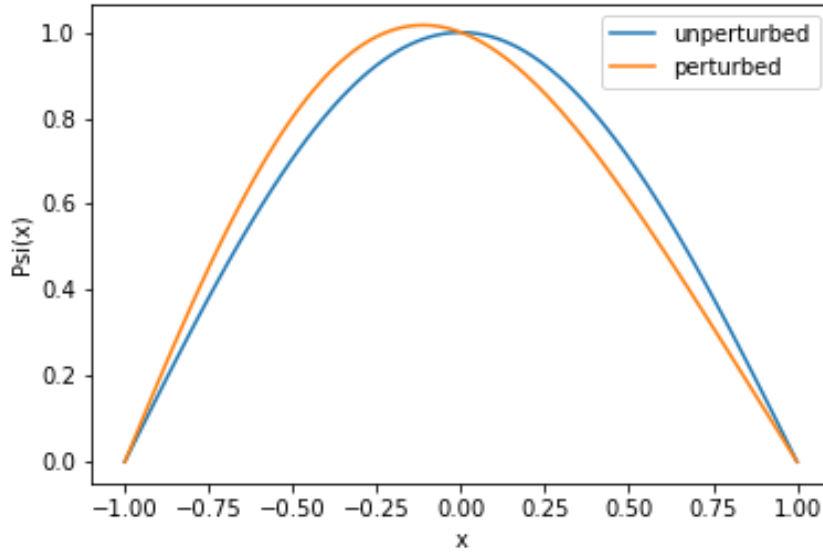


Figure 1: Perturbed vs unperturbed wave function for a 1D infinite square well of size $-a, \leq x \leq a$ where $a = 1$, perturbed by energy $V_1(x) = \lambda x/a$. We see that the perturbation shifts the wave function closer to one side of the well.

3. (6 points) **Townsend 11.16** In order to evaluate $\langle 1/r \rangle$ consider γ/r as a perturbation for the hydrogenic atom, where we can think of γ as some small constant. The first-order shift in the energy is given by

$$E_n^{(1)} = \left\langle \frac{\gamma}{r} \right\rangle_{n,l,m} \quad (21)$$

which is clearly linear in γ .

- (a) First show that the exact eigenvalues are given by

$$E_n = -\frac{\mu(Ze^2 - \gamma)^2}{2\hbar^2 n^2} \quad (22)$$

Solution: Writing down the Hamiltonian for this perturbed system:

$$\hat{H} = \frac{\hat{p}^2}{2m} - \frac{Ze^2}{r} + \frac{\gamma}{r} \quad (23)$$

Grouping $1/r$ terms we can write this as:

$$\hat{H} = \frac{\hat{p}^2}{2m} - \frac{(Ze^2 - \gamma)}{r} \quad (24)$$

Notice this is the exact same form as the unperturbed Hamiltonian with some pseudo-variable $\xi = Ze^2 - \gamma$. Thus we can get the energy by simply looking at the unperturbed result and substituting in our pseudo-vector:

$$E_n = -\frac{\mu(Ze^2 - \gamma)^2}{2\hbar^2 n^2} \quad (25)$$

to obtain the exact eigenvalue.

- (b) Since $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \dots$ we can obtain $E_n^{(1)}$ either by explicitly finding the contribution to E_n that is linear in γ , or, more generally, noting that

$$E_n^{(1)} = \gamma \left(\frac{dE_n}{d\gamma} \right)_{\gamma=0} \quad (26)$$

since $E_n^{(0)}$ is of course independent of γ and the higher order terms in the expansion are at least of order γ^2 . In this way, show that

$$\left\langle \frac{1}{r} \right\rangle_{n,l,m} = \frac{\mu Ze^2}{\hbar^2 n^2} = \frac{Z\mu c\alpha}{\hbar n^2} = \frac{z}{a_0 n^2} \quad (27)$$

Solution: Using the above relations

$$\left\langle \frac{1}{r} \right\rangle_{n,l,m} = \left(\frac{dE_n}{d\gamma} \right)_{\gamma=0} \quad (28)$$

From our result for E_n in part (a):

$$\left(\frac{dE_n}{d\gamma} \right) = \frac{d}{d\gamma} - \frac{\mu(Ze^2 - \gamma)^2}{2\hbar^2 n^2} = -\frac{\mu Ze^2 - \gamma}{2\hbar^2 n^2} (-2) \quad (29)$$

Letting $\gamma = 0$:

$$\left\langle \frac{1}{r} \right\rangle_{n,l,m} = \frac{\mu Ze^2}{\hbar^2 n^2} \quad (30)$$

as desired.

APPENDIX

```
import numpy as np
import matplotlib.pyplot as plt
```

```
#There are multiple ways of plotting and computing these functions ,
#this is just one example.
```

```
#Define the unperturbed wave function in the ground state n = 1
def unperturbed_wf(x, a):
    return np.sqrt(1 / a) * np.cos(np.pi * x / (2 * a))
```

```
#Define the perturbed wave function for the ground state n = 1,
#for perturbation lam
def perturbed_wf(x, a, lam, m, hbar, N):
```

```
#Set the first term of the wavefunction
psi_0 = unperturbed_wf(x, a)
```

```

#Calculate the coefficient term in front of the sum
sum_coefficient = 16 * lam / np.pi**2 * (8 * m * a**2 / hbar**2)

#Begin computing the correction term for the perturbation
correction_term = 0

#Compute the sum term
for k in range(2, N):

    #Select even k
    if k % 2 == 0:
        perturbation = (-1)**(k / 2) * k / (1 - k**2)**3 *
            np.sin(k * np.pi * x / (2 * a))

        correction_term += perturbation

    #if k is odd we do not add anything
    else:
        correction_term += 0

    return psi_0 + sum_coefficient * correction_term

#Set up the parameters
a = 1
x = np.linspace(-a, a, 100) #size of the well
m = 1 #set to 1; not really important
hbar = 1 #set to 1; not really important
lam = 0.1 #pick how large the perturbation is
N = 10 #Pick how high you want the sum to go to

psi_1 = unperturbed_wf(x, a)
psi_2 = perturbed_wf(x, a, lam, m, hbar, N)

#Plot the result
plt.plot(x, psi_1, label='unperturbed')
plt.plot(x, psi_2, label='perturbed')
plt.xlabel('x')
plt.ylabel('Psi(x)')
plt.legend()
plt.savefig('Perturbation_Comparison')
plt.show()

```