

Griffiths Chapter 3 (2)

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Problem 3.16 Solve $(p - \langle p \rangle)\Psi = ia(x - \langle x \rangle)\Psi$ for $\Psi(x)$. Note that $\langle x \rangle$, $\langle p \rangle$, and a are real constants.

$$\begin{aligned}
 p\Psi &= [ia(x - \langle x \rangle) + \langle p \rangle] \Psi \\
 \frac{d\Psi}{dx} &= \frac{i}{\hbar} [ia(x - \langle x \rangle) + \langle p \rangle] \Psi \\
 \frac{d\Psi}{\Psi} &= \left[-\frac{a}{\hbar}(x - \langle x \rangle) + \frac{i\langle p \rangle}{\hbar} \right] dx \\
 \int \frac{1}{\Psi} d\Psi &= \int \left[-\frac{a}{\hbar}(x - \langle x \rangle) + \frac{i\langle p \rangle}{\hbar} \right] dx \\
 \ln \Psi &= -\frac{a}{2\hbar}(x - \langle x \rangle)^2 + \frac{i\langle p \rangle x}{\hbar} + C \\
 \Psi(x) &= \exp(C) \exp\left(-\frac{a}{2\hbar}(x - \langle x \rangle)^2\right) \exp\left(\frac{i\langle p \rangle x}{\hbar}\right) \\
 &= A \exp\left(-\frac{a}{2\hbar}(x - \langle x \rangle)^2\right) \exp\left(\frac{i\langle p \rangle x}{\hbar}\right)
 \end{aligned}$$

Problem 3.18 Test the energy-time uncertainty principle for the wave function in Problem 2.5 and the observable x , by calculating σ_H , σ_x , and $d\langle x \rangle / dt$ exactly.

The wave function in Problem 2.5 is given by

$$\Psi(x, t) = \frac{\sqrt{2}}{2} [\psi_1(x)\varphi_1(t) + \psi_2(x)\varphi_2(t)], \text{ where } \psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \text{ and } \varphi_n(t) = \exp(-in^2\omega t)$$

or more simply

$$\Psi(x, t) = \frac{1}{\sqrt{a}} \left[\sin\left(\frac{\pi x}{a}\right) \exp(-\omega t) + \sin\left(\frac{2\pi x}{a}\right) \exp(-4\omega t) \right],$$

and solving for the probability density function we get

$$\rho(x) = |\Psi(x, t)|^2 = \frac{1}{a} \left[\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2 \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right) \cos(3\omega t) \right].$$

Note that all of the above was done in the 2nd homework assignment. For more detailed steps please refer to that.

Since σ_Q is given by $\sqrt{\langle Q^2 \rangle - \langle Q \rangle^2}$ for any operator Q , we will first have to find some expectation values.

$\langle x \rangle$ was shown in the 2nd assignment to be

$$\langle x \rangle = \frac{a}{2} - \frac{16a}{9\pi^2} \cos(3\omega t),$$

and $d\langle x \rangle / dt$ was shown to be

$$\frac{d\langle x \rangle}{dt} = \frac{8\hbar}{3ma} \sin(3\omega t).$$

Now we will find $\langle x^2 \rangle$

$$\begin{aligned}\langle x^2 \rangle &= \langle \Psi | x^2 \Psi \rangle = \int_0^a x^2 \rho(x) dx = \frac{1}{a} \int_0^a x^2 \left[\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2 \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right) \cos(3\omega t) \right] dx \\ &= \frac{1}{a} \left[\int_0^a x^2 \sin^2\left(\frac{\pi x}{a}\right) dx + \int_0^a x^2 \sin^2\left(\frac{2\pi x}{a}\right) dx + 2 \cos(3\omega t) \int_0^a x^2 \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right) dx \right]\end{aligned}$$

(integration done with SymPy and Wolfram|Alpha)

$$\begin{aligned}\langle x^2 \rangle &= \frac{1}{a} \left\{ \left[\frac{a^3}{6} - \frac{a^3}{4\pi^2} \right] + \left[\frac{a^3}{6} - \frac{a^3}{16\pi^2} \right] + 2 \cos(3\omega t) \left[-\frac{8a^3}{9\pi^2} \right] \right\} \\ &= \frac{a^3}{a} \left[\frac{1}{6} - \frac{1}{4\pi^2} + \frac{1}{6} - \frac{1}{16\pi^2} - 2 \cos(3\omega t) \frac{8}{9\pi^2} \right] = a^2 \left[\frac{1}{3} - \frac{5}{16\pi^2} - 2 \cos(3\omega t) \frac{8}{9\pi^2} \right]\end{aligned}$$

(note that $\text{lcm}(3, 16\pi^2, 9\pi^2) = 144\pi^2$)

$$\begin{aligned}\langle x^2 \rangle &= \frac{a^2}{144\pi^2} [48\pi^2 - 5 \cdot 9 - 2 \cos(3\omega t) 16 \cdot 8] = \frac{a^2}{144\pi^2} [48\pi^2 - 45 - 256 \cos(3\omega t)] \\ &= \left(\frac{a}{12\pi} \right)^2 [48\pi^2 - 45 - 256 \cos(3\omega t)]\end{aligned}$$

$$\langle x \rangle^2 = a^2 \left[\frac{1}{2} - \frac{16}{9\pi^2} \cos(3\omega t) \right]^2 = a^2 \left[\frac{1}{4} - \frac{16}{9\pi^2} \cos(3\omega t) + \left(\frac{16}{9\pi^2} \cos(3\omega t) \right)^2 \right]$$

$$\begin{aligned}\sigma_x^2 &= \langle x^2 \rangle - \langle x \rangle^2 = a^2 \left\{ \frac{48}{144} - \frac{45}{144\pi^2} - \frac{16}{9\pi^2} \cos(3\omega t) - \frac{1}{4} + \frac{16}{9\pi^2} \cos(3\omega t) + \left(\frac{16}{9\pi^2} \cos(3\omega t) \right)^2 \right\} \\ &= a^2 \left[\frac{1}{12} - \frac{5}{16\pi^2} + \left(\frac{16}{9\pi^2} \cos(3\omega t) \right)^2 \right]\end{aligned}$$

$\langle H \rangle$ was also found in the previous assignment, and has value

$$\langle H \rangle = \frac{5\pi^2 \hbar^2}{4ma^2}.$$

Now, instead of finding $\langle H^2 \rangle$, we can invoke Equation 3.21 to skip directly to σ_H .

$$\begin{aligned}\sigma_H^2 &= \langle (\hat{H} - \langle H \rangle) \Psi | (\hat{H} - \langle H \rangle) \Psi \rangle, \text{ where} \\ (\hat{H} - \langle H \rangle) &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \langle H \rangle \\ \sigma_H^2 &= \int_0^a \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} - \langle H \rangle \Psi^* \right) \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \langle H \rangle \Psi \right) dx \\ &= \int_0^a \left[\frac{\hbar^4}{4m^2} \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial^2 \Psi}{\partial x^2} + \langle H \rangle^2 \Psi^* \Psi + \langle H \rangle \Psi \frac{\hbar^2}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \langle H \rangle \Psi^* \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \right] dx \\ &= \frac{\hbar^4}{4m^2} \int_0^a \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial^2 \Psi}{\partial x^2} dx + \langle H \rangle^2 \int_0^a \Psi^* \Psi dx + \langle H \rangle \frac{\hbar^2}{2m} \int_0^a \Psi \frac{\partial^2 \Psi^*}{\partial x^2} dx + \langle H \rangle \frac{\hbar^2}{2m} \int_0^a \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx\end{aligned}$$

note that Ψ is real-valued, and therefore the complex conjugate is the identity function

$$\begin{aligned}\sigma_H^2 &= \frac{\hbar^4}{4m^2} \int_0^a \left(\frac{\partial^2 \Psi}{\partial x^2} \right)^2 dx + \langle H \rangle^2 \int_0^a \Psi(x)^2 dx + \langle H \rangle \frac{\hbar^2}{2m} \int_0^a \Psi \frac{\partial^2 \Psi}{\partial x^2} dx + \langle H \rangle \frac{\hbar^2}{2m} \int_0^a \Psi \frac{\partial^2 \Psi}{\partial x^2} dx \\ &= \frac{\hbar^4}{4m^2} \int_0^a \left(\frac{\partial^2 \Psi}{\partial x^2} \right)^2 dx + \langle H \rangle^2 + 2 \langle H \rangle \frac{\hbar^2}{2m} \int_0^a \Psi \frac{\partial^2 \Psi}{\partial x^2} dx\end{aligned}$$

using a computer algebra system I find the derivatives of Ψ , and evaluate the integrals

$$\begin{aligned}\frac{\partial^2 \Psi}{\partial x^2} &= -\frac{\pi^2}{\sqrt{a^5}} \left(\exp(3\omega t) + 8 \cos\left(\frac{\pi x}{a}\right) \right) \exp(-4\omega t) \sin\left(\frac{\pi x}{a}\right) \\ \int_0^a \left(\frac{\partial^2 \Psi}{\partial x^2} \right)^2 dx &= \frac{\pi^4}{a^5} \left(\frac{a}{2} \exp(6\omega t) + 8a \right) \exp(-8\omega t) \\ \int_0^a \Psi \frac{\partial^2 \Psi}{\partial x^2} dx &= -\frac{\pi^2}{a^3} \left(\frac{a}{2} \exp(6\omega t) + 2a \right) \exp(-8\omega t)\end{aligned}$$

plugging back into σ_H^2 and simplifying with a CAS, we get

$$\sigma_H^2 = \frac{\pi^4 \hbar^4}{16a^4 m^2} (25 \exp(8\omega t) - 8 \exp(6\omega t) - 8) \exp(-8\omega t)$$

Finally, we substitute σ_H and σ_x into the energy-time uncertainty principle

$$\begin{aligned}\Delta E = \sigma_H &= \sqrt{\frac{\pi^4 \hbar^4}{16a^4 m^2} (25 \exp(8\omega t) - 8 \exp(6\omega t) - 8) \exp(-8\omega t)} \\ &= \frac{\pi^2 \hbar^2}{4a^2 m} \sqrt{(25 \exp(8\omega t) - 8 \exp(6\omega t) - 8) \exp(-8\omega t)} \\ \Delta t = \frac{\sigma_x}{|d\langle x \rangle / dt|} &= a \sqrt{\frac{1}{12} - \frac{5}{16\pi^2} + \left(\frac{16}{9\pi^2} \cos(3\omega t) \right)^2} \frac{3ma}{8\hbar} \frac{1}{\sin(3\omega t)}\end{aligned}$$

We want to show that $\Delta E \Delta t \geq \hbar/2$, but I've run out of time to show this. Hopefully taking that product would simplify to something which can be shown to be at least $\hbar/2$.

Problem 3.31 Virial theorem. Use Equation 3.71 to show that

$$\frac{d}{dt} \langle xp \rangle = 2 \langle T \rangle - \left\langle x \frac{dV}{dx} \right\rangle,$$

where T is the kinetic energy ($H = T + V$). In a *stationary* state the left side is zero (why?) so

$$2 \langle T \rangle = \left\langle x \frac{dV}{dx} \right\rangle.$$

This is called the **virial theorem**. Use it to prove that $\langle T \rangle = \langle V \rangle$ for stationary states of the harmonic oscillator, and check that this is consistent with the results you got in Problems 2.11 and 2.12.

Equation 3.71 states that

$$\frac{d}{dt} \langle Q \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{Q}] \rangle + \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle$$

By inspecting the equation we are seeking to solve, $Q = xp$, and $\hat{Q} = x\hat{p}$. We will begin by expanding $[\hat{H}, x\hat{p}]$. First, recall that

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad \text{and} \quad \hat{H} = \frac{\hat{p}^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x).$$

By the definition of the commutator, it follows that

$$\begin{aligned} [\hat{H}, x\hat{p}](f) &= \hat{H}x\hat{p}(f) - x\hat{p}\hat{H}(f) \\ &= \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) x \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) (f) - x \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) (f) \\ &= \frac{\hbar}{i} \left[\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) x \left(\frac{\partial f}{\partial x} \right) - x \left(\frac{\partial}{\partial x} \right) \left(-\frac{\hbar^2}{2m} \frac{\partial^2 f}{\partial x^2} + V(x)f(x) \right) \right] \\ &= \frac{\hbar}{i} \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \left(x \frac{\partial f}{\partial x} \right) + xV(x) \frac{\partial f}{\partial x} + x \frac{\hbar^2}{2m} \frac{\partial^3 f}{\partial x^3} - x \frac{\partial}{\partial x} (V(x)f(x)) \right] \\ &= \frac{\hbar}{i} \left[-\frac{\hbar^2}{2m} \left(2 \frac{\partial^2 f}{\partial x^2} + x \frac{\partial^3 f}{\partial x^3} \right) + xV(x) \frac{\partial f}{\partial x} + x \frac{\hbar^2}{2m} \frac{\partial^3 f}{\partial x^3} - x \frac{\partial V}{\partial x} f(x) - xV(x) \frac{\partial f}{\partial x} \right] \\ &= \frac{\hbar}{i} \left[-\frac{\hbar^2}{m} \frac{\partial^2 f}{\partial x^2} - x \frac{\partial V}{\partial x} f(x) \right] \end{aligned}$$

now we remove the test

$$[\hat{H}, x\hat{p}] = \frac{\hbar}{i} \left[-\frac{\hbar^2}{m} \frac{\partial^2}{\partial x^2} - x \frac{\partial V}{\partial x} \right]$$

and substitute back into Equation 3.71

$$\begin{aligned} \frac{d}{dt} \langle xp \rangle &= \frac{i}{\hbar} \left\langle -\frac{\hbar}{i} \left(\frac{\hbar^2}{m} \frac{\partial^2}{\partial x^2} + x \frac{\partial V}{\partial x} \right) \right\rangle + \left\langle \frac{\partial (x\hat{p})}{\partial t} \right\rangle \\ &= \left\langle -\frac{\hbar^2}{m} \frac{\partial^2}{\partial x^2} \right\rangle - \left\langle x \frac{\partial V}{\partial x} \right\rangle + \left\langle \frac{\partial (x\hat{p})}{\partial t} \right\rangle \\ &= 2 \langle T \rangle - \left\langle x \frac{\partial V}{\partial x} \right\rangle + \left\langle \frac{\partial (x\hat{p})}{\partial t} \right\rangle \end{aligned}$$

In the typical case, the operator \hat{Q} does not depend on time, and therefore we can neglect the time derivative of $x\hat{p}$, leaving us with the desired result:

$$\frac{d}{dt} \langle xp \rangle = 2 \langle T \rangle - \left\langle x \frac{\partial V}{\partial x} \right\rangle.$$

In a stationary state, *nothing* depends on time, and therefore the time derivative of the expectation value of xp is zero, leaving us with

$$2 \langle T \rangle = \left\langle x \frac{\partial V}{\partial x} \right\rangle.$$

The harmonic oscillator has potential $V(x) = m\omega^2 x^2/2$, and so $\frac{dV}{dx} = m\omega^2 x$, meaning $\langle x \frac{dV}{dx} \rangle = \langle m\omega^2 x^2 \rangle = \langle 2V \rangle$, therefore $2\langle T \rangle = 2\langle V \rangle$, or simply $\langle T \rangle = \langle V \rangle$.

Problem 3.38 The Hamiltonian for a certain three-level system is represented by the matrix

$$\mathbf{H} = \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

Two other observables, A and B , are represented by the matrices

$$\mathbf{A} = \lambda \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \mathbf{B} = \mu \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

where ω , λ , and μ are positive real numbers.

- a. Find the eigenvalues and (normalized) eigenvectors of \mathbf{H} , \mathbf{A} , and \mathbf{B} .

(Note that all eigenvalues and eigenvectors were found with the assistance of `numpy.linalg.eig`)

\mathbf{H} has eigenvalues $E_1 = \hbar\omega$, $E_2 = E_3 = 2\hbar\omega$, and eigenvectors $|H_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|H_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, and $|H_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

\mathbf{A} has eigenvalues $a_1 = \lambda$, $a_2 = -\lambda$, $a_3 = 2\lambda$, and eigenvectors $|A_1\rangle = (1/\sqrt{2})\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|A_2\rangle = (1/\sqrt{2})\begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix}$, $|A_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

\mathbf{B} has eigenvalues $b_1 = \mu$, $b_2 = -\mu$, $b_3 = 2\mu$, and eigenvectors $|B_1\rangle = (1/\sqrt{2})\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$, $|B_2\rangle = (1/\sqrt{2})\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$, $|B_3\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$.

- b. Suppose the system starts out in the generic state

$$|\mathcal{S}(0)\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix},$$

with $|c_1|^2 + |c_2|^2 + |c_3|^2 = 1$. Find the expectation values (at $t = 0$) of H , A , and B .

$$\begin{aligned} \langle H \rangle &= \langle \mathcal{S}(0) | H | \mathcal{S}(0) \rangle = (c_1^* \ c_2^* \ c_3^*) \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \\ &= \hbar\omega (c_1^* \ c_2^* \ c_3^*) \begin{pmatrix} c_1 \\ 2c_2 \\ 2c_3 \end{pmatrix} = \hbar\omega (|c_1|^2 + 2(|c_2|^2 + |c_3|^2)) \\ \text{recall: } 1 &= |c_1|^2 + |c_2|^2 + |c_3|^2 \implies 1 - |c_1|^2 = |c_2|^2 + |c_3|^2 \\ \langle H \rangle &= \hbar\omega (|c_1|^2 + 2(1 - |c_1|^2)) = \hbar\omega (2 - |c_1|^2), \\ \langle A \rangle &= \langle \mathcal{S}(0) | A | \mathcal{S}(0) \rangle = (c_1^* \ c_2^* \ c_3^*) \lambda \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \\ &= \lambda (c_1^* \ c_2^* \ c_3^*) \begin{pmatrix} c_2 \\ c_1 \\ 2c_3 \end{pmatrix} = \lambda (c_1^* c_2 + c_2^* c_1 + 2|c_3|^2), \\ \langle B \rangle &= \langle \mathcal{S}(0) | B | \mathcal{S}(0) \rangle = (c_1^* \ c_2^* \ c_3^*) \mu \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \\ &= \mu (c_1^* \ c_2^* \ c_3^*) \begin{pmatrix} 2c_1 \\ c_3 \\ c_2 \end{pmatrix} = \mu (2|c_1|^2 + c_2^* c_3 + c_3^* c_2). \end{aligned}$$

- c. What is $|\mathcal{S}(t)\rangle$? If you measured the energy of this state (at time t), what values might you get, and what is the probability of each? Answer the same questions for A and for B .

We obtain $|\mathcal{S}(t)\rangle$ by writing $|\mathcal{S}(0)\rangle$ as a linear combination of time-independent eigenstates, and then tacking on the time dependence, $\exp(-iE_n t/\hbar)$.

One can intuitively write $|\mathcal{S}(0)\rangle$ as a linear combination of H 's eigenvectors, given by

$$|\mathcal{S}(0)\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} c_1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ c_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ c_3 \end{pmatrix} = c_1 |H_1\rangle + c_2 |H_2\rangle + c_3 |H_3\rangle.$$

Then by tacking on the time-dependence we obtain $|\mathcal{S}(t)\rangle$

$$|\mathcal{S}(t)\rangle = c_1 |H_1\rangle \exp(-iE_1 t/\hbar) + c_2 |H_2\rangle \exp(-iE_2 t/\hbar) + c_3 |H_3\rangle \exp(-iE_3 t/\hbar).$$

If you were to measure the energy of the state, there is a probability $|c_1|^2$ that you would observe $E_1 = \hbar\omega$, and a probability $|c_2|^2 + |c_3|^2$ that you would observe $E_2 = E_3 = 2\hbar\omega$.