Problem Set 4
CHM 305, Fall 2023

Distributed: Thursday, October 5, 2023
Due: Thursday, October 12, 2023 @ 5 PM ET

Problem Set Submission: Please submit assignment by uploading your files to Canvas. You may upload scanned handwritten work or digital documents as .pdf files.

Collaboration: Students are encouraged to interact with one another and to collaborate in learning and understanding the course material and homework problems. However, each student's assignments are expected to be their own work, reflecting their own understanding of the course material.

1 Commutators and Uncertainty Relations

(a) Evaluate the commutator $\left[\frac{d}{dx}, \frac{1}{x}\right]$ by applying the operators to an arbitrary function $f(x)$.

(b) Can the position and kinetic energy of an electron along the x axis be measured simultaneously to arbitrary precision? Why or why not? Consider the commutator of the corresponding quantum operators.

(c) Prove the following commutator identity:

$$\left[\hat{A} + \hat{B}, \hat{C}\right] = \left[\hat{A}, \hat{C}\right] + \left[\hat{B}, \hat{C}\right]$$

(d) Prove the following commutator identity:

$$\left[\hat{A}\hat{B}, \hat{C}\right] = \hat{A}\left[\hat{B}, \hat{C}\right] + \left[\hat{A}, \hat{C}\right]\hat{B}$$

(e) Prove that two non-commuting operators $\hat{A}$ and $\hat{B}$ cannot have a complete set of common eigenfunctions. *Hint:* Show that if $\hat{A}$ and $\hat{B}$ have a complete set of common eigenfunctions, then $\left[\hat{A}, \hat{B}\right]\psi = 0$ for any wavefunction ψ.

2 Particle-in-a-Box Uncertainties

(a) Calculate $\langle x \rangle$, $\langle x^2 \rangle$, $\langle p \rangle$, and $\langle p^2 \rangle$ tor the n^{th} 1D particle-in-a-box eigenfunction.

Note: You may already have evaluated some of these quantities in a previous problem set. No need to redo any calculations, just write down any result derived previously and reference where it came from.

You may use any trigonometric integrals or identities given in this problem set or on any previous problem set. You can also reference the list of integrals and identities posted on Canvas. Another useful integral may be:

$$\int x^2 \sin^2(\alpha x) dx = \frac{x^3}{6} - \left(\frac{x^2}{4\alpha} - \frac{1}{8\alpha^3} \right) \sin(2\alpha x) - \frac{x \cos(2\alpha x)}{4\alpha^2}$$

(b) Using your results from part (a), calculate $\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ and $\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$.

(c) Check that the uncertainty principle is satisfied for each $\psi_n(x)$. In other words, check whether $\sigma_x \sigma_p \geq \hbar/2$ for each n.

(d) Which eigenfunction of the PIB comes closest to the uncertainty limit?

3 Quantum Harmonic Oscillator Wavefunctions

The first few eigenfunctions of the quantum harmonic oscillator are

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

$$\psi_1(x) = \left(\frac{4\alpha^3}{\pi}\right)^{1/4} x\, e^{-\alpha x^2/2}$$

$$\psi_2(x) = \left(\frac{\alpha}{4\pi}\right)^{1/4} (2\alpha x^2 - 1)\, e^{-\alpha x^2/2}$$

recalling that we defined $\alpha \equiv \left(\frac{k\mu}{\hbar^2}\right)^{1/2}$ for compactness.

(a) Sketch $\psi_0(x)$, $\psi_1(x)$, and $\psi_2(x)$.

(b) In class, we verified that the ground state wavefunction $\psi_0(x)$ satisfied the Schrödinger equation. Verify that $\psi_1(x)$ satisfies the Schrödinger equation as well.

(c) Recall that eigenfunctions of the same Hamiltonian should be mutually orthogonal. Show that $\psi_0(x)$ is orthogonal to both $\psi_1(x)$ and $\psi_2(x)$ by explicit integration. *Hint:* Consider the useful properties of even and odd integrands:

$$\int_{-\infty}^{\infty} f(x)dx = 0 \qquad \text{for } f(x) \text{ odd}$$

$$\int_{-\infty}^{\infty} f(x)dx = 2\int_{0}^{\infty} f(x)dx \qquad \text{for } f(x) \text{ even}$$

The following Gaussian integrals may also come in handy, where n represents a positive integer:

$$\int_0^\infty e^{-\alpha x^2} dx = \left(\frac{\pi}{4\alpha}\right)^{1/2} \tag{1}$$

$$\int_0^\infty x^{2n} e^{-\alpha x^2} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{2^{n+1}\alpha^n} \left(\frac{\pi}{\alpha}\right)^{1/2} \tag{2}$$

$$\int_0^\infty x^{2n+1} e^{-\alpha x^2} dx = \frac{n!}{2\alpha^{n+1}} \tag{3}$$

Note: Use Eqn. (2) for even powers of x, and Eqn. (3) for odd powers of x.

4 Expectation Values and Uncertainties for the Quantum Harmonic Oscillator

(a) Compute $\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$, and $\langle p^2 \rangle$ for the $\psi_0(x)$ ground state of the quantum harmonic oscillator given in the previous problem. Use symmetry when you can, but carry out explicit integration where needed.

(b) Check the uncertainty principle for the $\psi_0(x)$ HO state by examining $\sigma_x \sigma_p$. Where does this quantity fall compared to the position-momentum uncertainty limit of $\hbar/2$ that we derived in class?

(c) Compute the expectation values of the kinetic energy and potential energy for the $\psi_0(x)$ HO state, by evaluating:

$$\langle KE \rangle = \left\langle \frac{p^2}{2m} \right\rangle$$

$$\langle V \rangle = \left\langle \frac{1}{2} k x^2 \right\rangle$$

(d) Is the sum of $\langle KE \rangle$ and $\langle V \rangle$ what you would expect?

5 The Time-Dependent Harmonic Oscillator

A particle in a harmonic oscillator potential starts out in the initial superposition state

$$\Psi(x, 0) = A \left[3\psi_0(x) + 4\psi_1(x) \right]$$

(a) Find A to normalize the wavefunction.

(b) Write down expressions for $\Psi(x, t)$ and $|\Psi(x, t)|^2$.

You will find that $|\Psi(x, t)|^2$ oscillates at exactly the classical harmonic oscillator frequency! That's interesting, but consider: what frequency would the system have oscillated at had we specified $\psi_2(x)$ in the initial superposition state instead of $\psi_1(x)$?

(c) If you measured the energy of this particle, what values might you measure, and with what probabilities?