2.11: Problems

1. Consider the functions $f(x) = A\left(1 - x^2\right)$ and $g(x) = 3x^3 - x$.
   a. Find a value for A such that $f(x)$ is normalized on the interval $-1 \leq x \leq 1$.
   b. Are the functions $\mathrm{f}(\mathrm{x})$ and $\mathrm{g}(\mathrm{x})$ orthogonal over the interval $-1 \leq \mathrm{x} \leq 1$?
2. Consider each of the following functions and the associated intervals. Indicate whether or not the given function is suitable as a wavefunction over the given interval.
   a. $\mathrm{e}^{\mathrm{x}} \qquad 0 \leq x \leq \infty$
   b. $\mathrm{e}^{-\mathrm{x}} \qquad 0 \leq x \leq \infty$
   c. $1/\mathrm{x} \qquad -\infty \leq \mathrm{x} \leq \infty$
   d. $\mathrm{e}^{\mathrm{i}\theta} \qquad 0 \leq x \leq 2\pi$
   e. $x(1-x) \qquad 0 \leq x \leq 1$
3. Consider the following operators. Determine whether or not they are Hermitian.
   a. d/dx
   b. $i\ \mathrm{d}/\mathrm{dx}$
   c. $\mathrm{d}^2/\mathrm{dx}^2$
   d. $i\ \mathrm{d}^2/\mathrm{dx}^2$
4. Consider an operator $\hat{\mathrm{A}}$ and associated set of eigenfunctions ϕ_{n} that satisfies

$$\hat{A}\phi_{\mathrm{n}} = a_{\mathrm{n}}\phi_{\mathrm{n}}$$

Show that if the operator is Hermitian that the eigenvalues a_{n} must be real-valued.

5. Consider the data in the table.
   a. Calculate $\langle x\rangle$ and $\left\langle x^2\right\rangle$.
   b. Calculate σ_x^2 for the data set.
   c. Does $\sigma_x^2 = \left\langle x^2\right\rangle - \langle x\rangle^2$? If not, what is the difference?
6. Consider a particle of mass m in a rectangular solid box with edge lengths given by $a = \mathrm{a}$, $b = 2\mathrm{a}$, $c = 2\mathrm{a}$. Find the degeneracies of the first 10 energy levels for the system.

i	x
1	2.3
2	6.4
3	4.2
4	3.5
5	4.9

7. Consider a particle of mass m that is in a one-dimensional box of length a. The system is prepared so that the wavefunction is given by $\psi(x) = \mathrm{Ax}(a-x)$.
   a. Find a value of A that normalizes the wavefunction.
   b. Find the expectation values for x and x^2 ($\langle x\rangle$ and $\langle x^2\rangle$).
   c. Find the expectation values for p and p^2 ($\langle \mathrm{p}\rangle$ and $\langle \mathrm{p}^2\rangle$).
   d. Given that the variance for a measurement is given by $\sigma_a^2 = \langle a^2\rangle - \langle a\rangle^2$ calculate the variances σ_{x}^2 and σ_{p}^2.
   e. Find the value of $\sigma_x\sigma_p$. Does it exceed $\frac{\hbar}{2}$?
8. Consider a particle of mass m in a box of length a. The system is prepared such that the wavefunction is given by $\psi(\mathrm{x}) = \mathrm{Ax}^2(a-\mathrm{x})$.
   a. Find a value of A that normalizes the wavefunction.
   b. What are the units on the wavefunction?
   c. Find $\langle x\rangle$.

d. Is $\langle x\rangle = a/2$? Why or why not?

9. Consider the following pairs of operators and determine whether or not the operators commute.
   a. $d/dx, d^2/dx^2$
   b. $x, d^2/dx^2$
   c. $x, \int dx$
10. Consider a particle of mass m in a box of length a for which the wavefunction is given by

$$\Psi(x) = (2)^{1/2}/3\phi_1(x) - (7)^{1/2}/3\phi_3(x)$$

where $\phi_n(x) = (2/a)^{1/2}\sin(n\pi x/a)$.

   a. Show that the wavefunction $\Psi(x)$ is normalized.
   b. Graph the wavefunction $\Psi(x)$.
   c. What is the expectation value for energy $\langle E\rangle$ for the system?
   d. What is the most likely energy to be measured for the system?
11. Consider benzene (C_6H_6) as modeled using the free-electron model.
   a. Using a $C-C$ bond length of $r_{cc} = 0.139$ nm, calculate the circumference of the ring and its radius.
   b. Based on the model, what are the degeneracies of the four lowest energy levels?
   c. Placing two electrons per particle-on-a-ring "orbital", calculate the energy gap (and corresponding wavelength of light driving a transition) between the HOMO and the LUMO based on this model.
   d. How does the value you found in part c compare to the observed band-origin of the $A_{1g} \rightarrow B_{1u}$ transition of benzene $(\lambda = 215 \text{ nm})$?