Worksheet 7.

1. **Explain, in one or two sentences and (hopefully) a diagram, what Compton Scattering is. Why was the observation of Compton scattering important to the development of quantum mechanics?**

2. An experimental study of the photoelectric effect is performed on a sample of Chromium, which has the work function $\Phi = 4.40 \text{ eV}$ and electrons with a kinetic energy of $2.88 \cdot 10^{-19} \text{ J}$ are emitted. **What is the wavelength of the light that is shining on the Chromium surface?**

3. **What is the momentum of a photon of the characteristic yellow light (589.3 nm) emitted by a sodium vapor lamp.**

4. **Which of the following are <u>not</u> linear, Hermitian, operators?**
   (a) $\frac{d}{dx}$ (the derivative)
   (b) $\frac{d^2}{dx^2}$ (2nd derivative)
   (c) $\frac{d^4}{dx^4}$ (4th derivative)
   (d) $g_+(x) = f(x) + f^*(x)$ (multiplication by $g_+(x)$, where $f(x) \in \mathbb{C}$ is any complex-valued function.
   (e) $g_-(x) = f(x) - f^*(x)$ (multiplication by $g_-(x)$, where $f(x) \in \mathbb{C}$ is any complex-valued function.
   (f) $g(x) = f(x)\, f^*(x)$ (multiplication by $g(x)$, where $f(x) \in \mathbb{C}$ is any complex-valued function.
   (g) $ig(x) = if(x)\, f^*(x)$ (multiplication by $ig(x)$, where $f(x) \in \mathbb{C}$ is any complex-valued function.
   (h) $\ln(\quad)$ (the operator that takes the natural logarithm of a function.

5. **What is the probability of observing a particle in the first quarter of a box of length *a*. That is, write and evaluate an expression for the probability that a particle-in-a-box is located between zero and *a*/4.**

The following text is relevant to problems 6-9.
One of the key steps in quantum computing is to carefully prepare systems so that we have the wavefunction that is needed to do the "computation." Suppose we tried to build a quantum computer based on the particle-in-a-box. Assume that the particle has unit mass, the box has unit length, and that the "walls" of the box are infinitely high. So

$$V(x) = \begin{cases} 0 & 0 < x < 1 \\ +\infty & \text{otherwise} \end{cases} \tag{1}$$

After a careful preparation, the wavefunction is expanded in terms of the eigenfunctions of the particle in a box,

$$\Psi(x,t) = 3\psi_1(x,t) + 4\psi_2(x,t) + 5\psi_3(x,t) \tag{2}$$

where $\psi_n(x,t)$ are the normalized eigenfunctions of the particle-in-a-box.

6. **Is $\Psi(x,t)$ normalized?**

7. **What is the expectation value of the energy for $\Psi(x)$?**

8. **What is the probability of finding the system in the *n=3* state?**

9. A stationary state is a state where the probability of observing the particle at position x does not depend on the time. (I.e., $P(x,t) = P(x)$.) **Does $\Psi(x,t)$ describe a stationary state of the particle-in-a-box?**

10. Suppose that $\hat{A}$ and $\hat{B}$ are linear, Hermitian, operator. Consider the product of these matrices, raised to the n^{th} power:

$$\left(\hat{A}\hat{B}\right)^n = \underbrace{\left(\hat{A}\hat{B}\right)\left(\hat{A}\hat{B}\right)\cdots\left(\hat{A}\hat{B}\right)}_{n \text{ times}} \qquad n = 0,1,2,3,\ldots \tag{3}$$

(a) Show that

$$\left\langle \Phi \middle| \left(\hat{A}\hat{B}\right)^n \middle| \Psi \right\rangle = \left\langle \Phi \middle| \left(\hat{A}\hat{B}\right)^n \Psi \right\rangle = \left\langle \left(\hat{B}\hat{A}\right)^n \Phi \middle| \Psi \right\rangle \tag{4}$$

(b) Is the product of two Hermitian operators always Hermitian? If not, under what conditions is it true?

11. Suppose the Hamiltonian of a system does not depend on time. (I.e., $\hat{H}(x,t) \to \hat{H}(x)$.) **Starting from the time-dependent Schrödinger equation, derive the time-independent Schrödinger equation. Write an explicit formula for the time-dependent wavefunction in terms of the energy eigenvalue of the time-independent Schrödinger equation.**

12. Consider a particle of mass m confined to a two-dimensional rectangular box with potential,

$$V(x,y)=\begin{cases}0 & 0<x<a \text{ and } 0<y<b \\ +\infty & \text{otherwise}\end{cases} \tag{5}$$

   (a) Solve the time-independent Schödinger equation to find the eigenfunctions and the eigenvalues of this system. You should obtain:

$$\begin{aligned}\Psi_{n_x,n_y}(x,y) &= \frac{2}{\sqrt{ab}}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{b}\right)\\ E_{n_x n_y} &= \frac{h^2}{8m}\left(\frac{n_x^2}{a^2}+\frac{n_y^2}{b^2}\right)\\ n_x &= 1,2,3,\ldots\\ n_y &= 1,2,3,\ldots\end{aligned} \tag{6}$$

   (b) Suppose $b=3$ and $a=5$. **Write expressions for the transition frequencies associated with the <u>two lowest-energy</u> (lowest frequency) absorptions starting from the ground state.** (That is, the initial state is $m=n=1$).

13. The simplest model of molecular vibrations is the so-called Harmonic oscillator model. In the simple one-dimension harmonic oscillator, the bond between the atoms in a diatomic molecule is approximated as a spring, with force constant k_e and equilibrium bond length r_e. The resulting potential is simply a parabola, $V_{\text{HO}}(r)=\frac{1}{2}k_e(r-r_e)^2$. The eigenvalues of the simple oscillator are given by

$$E(\upsilon)=\hbar\left(\sqrt{\tfrac{k_e}{\mu}}\right)\left(\upsilon+\tfrac{1}{2}\right) \qquad \upsilon=0,1,2,\ldots \tag{7}$$

   where the reduced mass of the oscillator is simply related to the atomic masses by $\mu=\left(m_A m_B/(m_A+m_B)\right)$. The eigenfunctions of the three lowest energy states of the harmonic oscillator are given below

$$\begin{aligned}\psi_0(r)&=\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\frac{\alpha}{2}(r-r_e)^2} \qquad \psi_1(r)=\left(\frac{\alpha}{\pi}\right)^{1/4}\left(\sqrt{2\alpha}\right)(r-r_e)e^{-\frac{\alpha}{2}(r-r_e)^2}\\ \psi_2(r)&=\left(\frac{\alpha}{\pi}\right)^{1/4}\left(\frac{1}{\sqrt{8}}\right)\left(4\alpha(r-r_e)^2-2\right)e^{-\frac{\alpha}{2}(r-r_e)^2}\end{aligned} \tag{8}$$

   where

$$\alpha=\sqrt{\frac{k_e\mu}{\hbar^2}} \tag{9}$$

   (a) Write down the Harmonic-Oscillator Hamiltonian and show that $\psi_0(r)$ is an eigenfunction of it.

   (b) What is the ground-state energy and the ground-state wavefunction of the "half-oscillator" (4 points)

$$V_{\frac{1}{2}\text{HO}}(r)=\begin{cases}V_{\text{HO}}(r)=\frac{1}{2}k_e(r-r_e)^2 & r_e\le r<+\infty \\ +\infty & -\infty<r<r_e\end{cases} \tag{10}$$