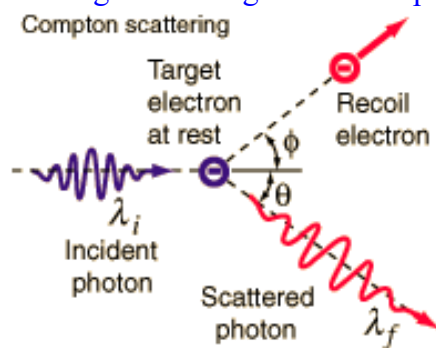


Worksheet 7. **KEY**

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?

Compton Scattering is where a photon “collides with” or “scatters off of” an electron. It allows one to measure the momentum of a photon, and was important in quantum mechanics because it helped clarify the “particle nature of light.” A diagram of Compton scattering is below.



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?** The energy of the light goes into the (a) work function and (b) the kinetic energy of the emitted electrons. So the energy of the light is

$$\begin{aligned} E_{\text{light}} &= h\nu = \Phi + T = 4.4 \text{ eV} + 2.88 \cdot 10^{-19} \text{ J} \\ &= 4.40 \text{ eV} \left( \frac{1.602 \cdot 10^{-19} \text{ J}}{1 \text{ eV}} \right) + 2.88 \cdot 10^{-19} \text{ J} \\ &= 9.929 \cdot 10^{-19} \text{ J} \end{aligned}$$

and the frequency of the light is:

$$\nu = \frac{9.929 \cdot 10^{-19} \text{ J}}{h} = \frac{9.929 \cdot 10^{-19} \text{ J}}{6.626 \cdot 10^{-34} \text{ J} \cdot \text{s}} = 1.498 \cdot 10^{15} \text{ Hz}$$

so the wavelength is

$$\lambda = \frac{c}{\nu} = \frac{2.998 \cdot 10^8 \frac{\text{m}}{\text{s}}}{1.498 \cdot 10^{15} \frac{1}{\text{s}}} = 2.001 \cdot 10^{-7} \text{ m} = 200 \text{ nm}.$$

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

Using the De Broglie relation,

$$p = \frac{h}{\lambda} = \frac{6.6262 \cdot 10^{-34} \text{ J} \cdot \text{s}}{589.3 \cdot 10^{-9} \text{ m}} = 1.124 \cdot 10^{-27} \frac{\text{kg} \cdot \text{m}}{\text{s}}$$

4. Which of the following are not linear, Hermitian, operators?

(a)  $\frac{d}{dx}$  (the derivative)

- (b) (2<sup>nd</sup> derivative)
- (c) (4<sup>th</sup> derivative)
- (d) (multiplication by  $g_+(x)$ , where is any complex-valued function.
- (e) (multiplication by  $g_-(x)$ , where is any complex-valued function.**
- (f) (multiplication by  $g(x)$ , where is any complex-valued function.
- (g) (multiplication by  $ig(x)$ , where is any complex-valued function.**
- (h) (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 integral is . For an eigenstate of the particle-in-a-box, this would be

.

**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

(11)

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

(12)

where are the normalized eigenfunctions of the particle-in-a-box.

## 6. Is normalized?

Let's start by computing the candidate probability distribution function,

We know that the eigenstates of any time-independent Hamiltonian can be written as and for the special case of the particle in a box, we have:

Thus we have:

and

If the spatial wavefunctions are real, like they are for the particle in a box, then:

So we have:

Substituting this expression into the normalization integral gives:

This wavefunction is not normalized.

## 7. What is the expectation value of the energy for ?

Evaluating

Using the fact that the mass and the length of the box are one, and the value of Planck's constant, we obtain

Given that we had a mass of 1 kg in a box of 1 meter (which is *very* classical), the tiny size of this number is not at all surprising.

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

It is just the square of the  $c_3$  coefficient in the *normalized* wavefunction. So:

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., .) **Does describe a stationary state of the particle-in-a-box?**  
No. Looking at the expression for it is clear that the probability is changing in time.

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

(13)

(a) Show that

(14)

$n = 0$ . The result is obviously true for  $n = 0$  because for any operator and .

$n = 1$ . The result is true for  $n = 1$  by the following argument, which uses the fact that  $A$  and  $B$  are Hermitian:

Now we want to show that if the result is true for one value of  $n$  greater than or equal to one, it is also true for  $n+1$ . That is, we want to show that if , then .

$n=k \rightarrow n=k+1$ :

This is called a proof by induction. The idea is that if you give me a value of  $n$  (say,  $n = 59$ ), then I know that the result is true if the result is true for  $n = 58$ . In turn, I know that the result for  $n = 58$  is true if the result is true for  $n = 57$ , and that the result for  $n = 57$  is true if the result is true for  $n = 56$ , and ..., and that the result is true for  $n = 2$  if the result is true for  $n = 1$ . But the result is true for  $n = 1$  (which was simple to show) so the result must also be true for  $n = 59$  and, by the same argument, for any  $n$  that is a nonnegative integer.

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

Clearly not, since the  $n=1$  case of Eq. **Error! Reference source not found.** indicates that . Obviously the product of two Hermitian operators is Hermitian if they commute, so that so that the last inequality is replaced by an equality.

11. Suppose the Hamiltonian of a system does not depend on time. (I.e., .) **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.**

If the Hamiltonian is time-independent, then replacing with in the time-dependent Schrödinger equation gives

Whenever you can “divide” a multidimensional differential equation into a sum of two terms, each of which has an explicit dependence on only a subset of the variables, you can simplify the differential equation by a technique called “separation of variables,” where you assume the solution can be written as a product of the a function of the “variables in the first part” and a function of the “variables in the second part.” In this case we have

and so we hypothesize a form of the wavefunction like

Substituting this wavefunction into the time-dependent Schrödinger equation gives

Divide both sides by . We obtain:

The left-hand-side depends only on  $x$ ; the right-hand-side depends only on  $t$ . However, the equation must hold for *all*  $x$  and  $t$ , which can happen only if this equation is equal to a constant. So we have:

or

Identifying the second equation as the time-independent Schrödinger equation, we see that the constant must be the energy. So

We can solve the ordinary differential equation for the time-dependent portion of the wavefunction by explicit integration,

It is obvious that the if  $\psi(x)$  is a solution to the Schrödinger equation, then any multiple of the wavefunction,  $C\psi(x)$ , is also. So we can ignore the constant of integration.



12. Consider a particle of mass  $m$  confined to a two-dimensional rectangular box with potential, (15)

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

(16)

The Hamiltonian is

and so the wavefunction must be zero outside the box,

When the Hamiltonian is the sum of two terms, each of which depends on only one variable, we should proceed by separation of variables. So we guess that the wavefunction is a product of a function of  $x$  and a function of  $y$ :

and substitute into the Schrödinger equation (inside the box) to obtain:

This equation indicates that sum of some function of  $x$  and some function of  $y$ , equals a constant for all permissible values of  $x$  and  $y$ .

This can only happen if the individual functions are constants also. This gives the equations:

but these equations are identical to the *one-dimensional* particle-in-a-box. So

and similarly

So the wavefunction is

and substituting in gives:

- (b) Suppose  $\psi_{11}$  and  $\psi_{21}$ . **Write expressions for the transition frequencies associated with the two lowest-energy (lowest frequency) dipole-allowed absorptions starting from the ground state.** (That is, the initial state is  $\psi_{11}$ ). (4 pts.)

The lowest-energy absorptions are

However, the second-lowest absorption (#2) is *not dipole allowed* because the transition is not allowed for the *one-dimensional* oscillator. (It also isn't allowed here, because  $\psi_{11}$  isn't changing.) This part of this problem is too advanced for "right now" but will make sense later.

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  $k$  and equilibrium bond length  $r_0$ . The resulting potential is simply a parabola,  $V = \frac{1}{2}k(r - r_0)^2$ . The eigenvalues of the simple oscillator are given by

(17)

where the reduced mass of the oscillator is simply related to the atomic masses by  $\mu = \frac{m_1 m_2}{m_1 + m_2}$ . The eigenfunctions of the three lowest energy states of the harmonic oscillator are given below

(18)

where

(19)

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

1. The Harmonic Oscillator Hamiltonian is

2.  $\psi_0$  is an eigenfunction of this Hamiltonian because:

(20)

(b) What is the ground-state energy and the ground-state wavefunction of the “half-oscillator”

(21)

Remember what we did for the particle in a box. We said that the eigenfunctions of the Hamiltonian were  $\psi_k$  for any  $k$ , but the fact that the potential was infinity for  $x=0$  and  $x=L$  meant that the wavefunction had to be zero at those two values,  $x=0$  and  $x=L$ . This case is similar. The solutions to the harmonic oscillator potential are given in the problem, but in the half-oscillator we also require that  $\psi(0)=0$ . So half of the solutions of the harmonic oscillator are no longer allowed (do not satisfy  $\psi(0)=0$ ). The new ground state is thus  $\psi_1$  and the ground-state energy is  $E_1$ .





