Physics Unlimited Explorer Competition

Assignment packet, revised 3/5/21

Submissions due: March 21, 2021 11:59 pm EST

Guidelines

Student teams will have a total of **up to two weeks** to work on the 2021 Explorer Competition, and teams registering later than the assignment release date may begin to work at any time. For successful completion of this assignment, we recommend that teams set aside at least 10 hours of time, cumulatively. Please refer to the submission explanation below for details on both formatting and the submission process.

Scoring

Students are encouraged to work on as much of the assignment as possible. The award structure will be as follows:

1. Certificate awards will be given to the four teams with the highest scores, per scoring rubric that would allocate points for questions and exercises based on their difficulty level as determined by the assignment creator.
2. There will be medalist certificates granted for first place, second place, and third place, respectively.
3. There will be an honorable mention certificate granted to the fourth-highest scoring submission.

Collaboration Policy and External Resources

Students participating in the competition **may only correspond with members of their team**. Absolutely and unequivocally, **no other form of human correspondence is allowed**. This includes any form of correspondence with mentors, teachers, professors, and other students. Participating students are barred from posting content or asking questions related to the exam on the internet (except where specified below), and moreover, they are unequivocally barred from seeking the solution to any of the exams' parts from the internet or another resource. Students are allowed, however, to use the following resources for purposes of reference and computation:

- **Internet**: Teams may use the internet for purposes of reference with appropriate citation. Again, teams are in no way allowed to seek the solution to any of the exams' parts from the internet. For information about appropriate citation, see below.
- **Books and Other Literature**: Teams may use books or other literature, in print or online, for purposes of reference with appropriate citation. As with the use of the Internet, teams are in no way allowed to seek the solution to any of the exams' parts from books or other literature.
- **Computational Software**: Teams may use computational software, e.g. Mathematica, Matlab, Python, whenever they deem it appropriate. Of course, teams must clearly indicate that they have used such software. Additionally, the judges reserve to right to deduct points for the use of computational software where the solution may be obtained simply otherwise.

Citation

All student submissions that include outside material must include numbered citations. We do not prefer any style of citation in particular.

Submission

All submissions, regardless of formatting, **should include a cover page listing the title of the work, the date, and electronic or scanned signatures of all team participants**. The work must be submitted as a single **PDF document** with the ".pdf." extension. All other formatting decisions are delegated to the teams themselves. No one style is favored over another. That being said, we recommend that teams use a typesetting language (e.g. LATEX) or a word-processing program (e.g. Microsoft Word, Pages). **Handwritten solutions are allowed**, but we reserve the right **to refuse grading of any portion of a team's submission in the case that the writing or solution is illegible**.

All teams must submit their solutions document to the 2021 Explorer Competition by **emailing directors@physicsu.org by 11:59 pm Eastern Time (UTC-5) on Sunday, March 21, 2021**. Teams will not be able to submit their solutions to the Explorer Competition at any later time. The team member who submitted the team registration form should send the submission; in case they are unable to, another team member may do so. The title of the submission e-mail should be formatted as **"PUEC 2021 SUBMISSION - Team Name"**, without quotation marks, where **Team Name** is to be replaced with your actual team's name, as registered. All teams may make multiple submissions. However, we will **only read and grade the most recent submission submitted before the deadline**. Teams will receive confirmation once their submission has been received within at most two days. **In the case of extraordinary circumstances, please contact us as soon as possible**.

Quantum Cascade Lasers

Contents

Learning Goals

Through the course of this assignment, you will learn some basic concepts and ideas about quantum mechanics and apply it to consider principles of designing a type of laser called a quantum-cascade laser. We want you to get an idea of the way fundamental physics concepts form the foundations of modern, cutting-edge technologies, and for you to see that even a little bit of physics knowledge can help you understand these devices a whole lot better.

Those of you who have worked on the 2018 Explorer assignment or looked over it while reviewing might find some of the content familiar. However, rest assured each question will be different.

Topic Format and Grading

This document consists of a few sections of expository material with exercises and questions interspersed along that lead you to considering several ideas related to laser design. Exercises will typically ask students to mathematically derive or demonstrate a result useful to the discussion. Questions will ask students to, in their own words, interpret stated results. We are looking to see how well you understand the subject, so to receive full credit, all work shown must be complete and properly justified.

Expected Amount of Work

Do not expect to understand the concepts in this document after only one read through; these concepts take time to absorb. While it may feel like you are not getting much accomplished as you try to understand the reading, persevere. It may be necessary to read some passages several times in a row before understanding them completely. Because there are not too many questions in this document, you should have time to complete the readings. We have made every attempt to be rigorous in our presentation, but simplifications have been made when appropriate. Students are welcome to investigate the subject in more detail outside of this document.

I Schrodinger's Equation

I.1 Introduction to Schrodinger's Equation

In classical mechanics, we describe the state of a particle using its position, velocity, acceleration, momentum, kinetic energy, and more. Classical mechanics says a particle has absolute, precise values for all of these quantities, and that in theory one could measure them all and know them all at the same time.

Quantum mechanics, on the other hand, describes the state of a particle using its **wavefunction**, $\Psi(\vec{r}, t)$. If the particle is confined to the x axis, then this simplifies to $\Psi(x, t)$. $\Psi(x, t)$ must satisfy **Schrodinger's equation**:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V\Psi(x,t) \tag{1}$$

where V is the potential energy of the system and $\hbar = h/(2\pi) = 1.054572 * 10^{-34}\, J$

$\Psi(x, t)$ can tell you many things about the system. For instance, the probability of finding the particle between positions $x = a$ and $x = b$ (for a particle moving only in the x direction) at time t is given by

$$p(x \text{ is between } a \text{ and } b) = \int_a^b \left|\Psi(x,t)\right|^2 dx$$

and $\left|\Psi(x,t)\right|^2$ gives the probability of finding the particle at point x at time t. In order to ensure that this is giving the probability, we must make sure that the sum of all the probabilities (or the integral, for continuous variables) adds up to 1 over all of space. In other words,

$$\int_{-\infty}^{\infty} \left|\Psi(x,t)\right|^2 dx = 1 \tag{2}$$

When $\Psi(x, t)$ fulfills this condition, we say it is properly **normalized**. Since the wavefunction can give us probabilities, we can use it to calculate **expectation values**. In probability, we can generalize the mean by using **probability distributions**. For example, if three people had the following ages: 23, 23, 24, then the mean age $\bar{a}$ would be

$$\bar{a} = \frac{23+23+24}{3} = \frac{1}{3}(23+23) + \frac{1}{3}(24) = \frac{2}{3} * 23 + \frac{1}{3} * 24 = 23.\bar{3}3$$

where the bar over the a is frequently used to denote averages. As you can see above, we were able to write the average in terms of the expression

$$\bar{a} = \sum_{j=0}^{\infty} jP(j) \text{ where } P(j) = \begin{cases} 2/3 & j = 23 \\ 1/3 & j = 24 \\ 0 & j \neq 23, 24 \end{cases}$$

We can generalize this sum for non-integers as well, and for continuous variables we would have integrals. In quantum mechanics, these averages are called **expectation values**, and are denoted as $\langle b \rangle$ for a variable b. For instance, for the continuous variable x, the average position $\langle x \rangle$ of a system in state $\Psi(x,t)$ would be

$$\langle x \rangle = \int_{-\infty}^{\infty} x \Big| \Psi(x,t) \Big|^2 dx = \int_{-\infty}^{\infty} \Psi^*(x,t) x \Psi(x,t)$$

The first half of the equality simply generalizes what we know about expectation values as sums weighted by the probabilities of a given outcome. The second half rewrites

$$\Big| \Psi(x,t) \Big|^2 = \Psi^*(x,t)\Psi(x,t)$$

since $\Psi((x,t)$ can be complex in general, and then sandwiches the x in between $\Psi^*(x,t)$ and $\Psi(x,t)$. In general, the right-hand side of the equality is how we want to write out expectation values. This is because in general, we will take expectation values of operators, which may or may not contain operations like derivatives that will act on $\Psi(x,t)$. For example, if we want to find the expectation value of momentum, we would write

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = m \int_{-\infty}^{\infty} x \frac{\partial}{\partial t} \Big| \Psi \Big|^2 dx$$

and then we can use the original time-dependent Schrodinger equation, Equation (1), to write

$$\langle p \rangle = m \int_{-\infty}^{\infty} x \frac{\partial}{\partial t} \Big| \Psi \Big|^2 dx = \frac{i\hbar}{2} \int_{-\infty}^{\infty} x \frac{\partial}{\partial x} \Big(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \Big) dx = \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi \, dx \quad (3)$$

I will skip over the mathematical details used in the intermediary stages of the equation above used to get to the right-hand side, which involve integration by parts. At risk of incurring your wrath, the proof of this result will be left as an exercise to the reader, as you will see in the **Exercises** section for this section. Hopefully, however, this is enough of an illustration to show why we **must** write expectation values as

$$\langle \hat{O} \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \hat{O} \Psi(x,t) \, dx$$

instead of

$$\int_{-\infty}^{\infty} \hat{O} \Big| \Psi(x,t) \Big|^2 dx$$

The $\hat{}$ above the O denotes an **operator**, which is a general expression used to denote an observable and can contain operations such as derivatives that act on a wavefunction. For instance, going back to the specific case of momentum, Equation (3) tells us that

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}, \;\; \langle \hat{p} \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi(x,t) \, dx \quad (4)$$

In the case of x, we simply have the operator $\hat{x} = x$, which is consistent with our expression for $\langle x \rangle$.

Finally a distribution of values also has a certain spread, called the **standard deviation**, that quantifies an average of how much each value deviates from the mean value of the distribution. We can write this as

$$\sigma \equiv \sqrt{\left\langle \left(j - \left\langle j \right\rangle\right)^2 \right\rangle} \text{ so that } \sigma^2 = \left\langle \left(j - \left\langle j \right\rangle\right)^2 \right\rangle$$

where σ^2 is called the **variance**. You will prove in one of the exercises that

$$\sigma^2 \equiv \left\langle \left(j - \left\langle j \right\rangle\right)^2 \right\rangle = \left\langle j^2 \right\rangle - \left\langle j \right\rangle^2 \tag{5}$$

Thus, we can calculate not only the expectation values of operators like $\hat{x}$ and $\hat{p}$, but we can also calculate their standard deviations σ_x and σ_p and see how much uncertainty there is. For example, writing variances to reduce notational clutter from square root symbols

$$\sigma_x^2 = \int_{-\infty}^{\infty} \Psi^*(x,t) x^2 \Psi(x,t)\, dx - \left(\int_{-\infty}^{\infty} \Psi^*(x,t) x \Psi(x,t)\, dx \right)^2 \tag{6}$$

$$\sigma_p^2 = \int_{-\infty}^{\infty} \Psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x}\right)^2 \Psi(x,t)\, dx - \left(\int_{-\infty}^{\infty} \Psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x}\right) \Psi(x,t)\, dx \right)^2 \tag{7}$$

In quantum mechanics, there is a relationship between σ_x and σ_p called the **uncertainty principle**:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \tag{8}$$

This tells us that we cannot measure both position and momentum with arbitrary precision each time (which would reduce the spread in the values of x and p) − the more precisely you know one, the less precisely you know the other. I encourage you to look into the proof for this principle for your own learning, but it will not be an exercise on this exam.

I.1.1 Exercise

Show the intermediary steps needed to fully illustrate Equation (3): in other words, show that

$$\left\langle \hat{p} \right\rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x}\right) \Psi(x,t)\, dx$$

for a general wavefunction $\Psi(x,t)$. To do this, you must do the following two things:

1. First, we will give you that

   $$\frac{d}{dt} \int_{-\infty}^{\infty} \left|\Psi(x,t)\right|^2 dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} \left|\Psi(x,t)\right|^2 dx$$

   since the left-hand side has the integral depending solely on time, allowing us to write a total time derivative outside the integral, but on the right-hand side $\left|\Psi(x,t)\right|^2$ depends on both x and t, so we need a partial derivative when pulling the derivative inside the integral.

   Using this, illustrate that

   $$\frac{d}{dt} \int_{-\infty}^{\infty} \left|\Psi(x,t)\right|^2 dx = \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \frac{\partial}{\partial x} \left(\Psi^*(x,t) \frac{\partial \Psi(x,t)}{\partial x} - \frac{\partial \Psi^*(x,t)}{\partial x} \Psi(x,t) \right) dx$$

   You will need Equation (1) for this.

2. Finish the proof by showing that

   $$\frac{i\hbar}{2} \int_{-\infty}^{\infty} x \frac{\partial}{\partial x} \left(\Psi^*(x,t) \frac{\partial \Psi(x,t)}{\partial x} - \frac{\partial \Psi^*(x,t)}{\partial x} \Psi(x,t) \right) dx = \int_{-\infty}^{\infty} \Psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x}\right) \Psi(x,t)\, dx$$

   using integration by parts.

   Hint: Assume $\Psi(x,t) \to 0$ as $x \to \pm\infty$ in order to be normalizable.

I.1.2 Exercise

Prove Equation (5): show that

$$\left\langle \left(j - \langle j \rangle\right)^2 \right\rangle = \langle j^2 \rangle - \langle j \rangle^2$$

Hint: Since $\langle j \rangle$ is a constant for a given distribution of j, we can pull it out of sums.

I.1.3 Exercise

Suppose the wavefunction of a system is given by

$$\psi(x) = \begin{cases} A \sin\left(\frac{\pi x}{a}\right) & 0 \leq x \leq a \\ 0 & x > a, \;\; x < 0 \end{cases}$$

1. Find the value of A such that the wavefunction is properly normalized and fulfills Equation (2).
2. Use this normalized wavefunction to calculate $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$, the expectation values of the position and momentum of a particle in this state.
3. Use the normalized wavefunction to calculate σ_x and σ_p using Equations (6) and (7) and confirm that it adheres to the uncertainty principle given by Equation (8).

I.2 Separation of Variables

We can use a trick called **separation of variables** to attempt to solve Schrodinger's equation when the potential V is time-independent ($V = V(x)$), in which we take

$$\Psi(x,t) = \psi(x)\phi(t)$$

which would give us

$$\frac{\partial \Psi(x,t)}{\partial t} = \psi(x)\frac{\partial \phi(t)}{\partial t} \text{ and } \frac{\partial^2 \Psi(x,t)}{\partial x^2} = \frac{\partial^2 \psi(x)}{\partial x^2}\phi(t)$$

that we can plug back into Equation (1) to get

$$i\hbar\psi(x)\frac{\partial \phi(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2}\phi(t) + V(x)\psi(x)\phi(t)$$

If we divide both sides by $\Psi(x,t) = \psi(x)\phi(t)$, then we get

$$i\hbar\frac{1}{\phi(t)}\frac{\partial \phi(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2 \psi(x)}{\partial x^2} + V(x)$$

Now, the left hand side of the equation above is only dependent on time t while the right hand side of the equation above is only dependent on position x. In order for this to be the case, both sides must equal a constant. If we call this constant E, then on the right-hand side we see that

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = E$$

and after multiplying both sides by $\psi(x)$, we get

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x) \tag{9}$$

Similarly, the left-hand side would give us

$$i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = E$$

and multiplying. both sides by $\phi(t)$ and dividing by $i\hbar$ would give us

$$\frac{\partial\phi(t)}{\partial t} = \frac{E}{i\hbar}\phi(t) = -\frac{iE}{\hbar}\phi(t)$$

where on the right-hand side I multiplied the numerator and denominator by i. This has the solution

$$\phi(t) = e^{-\frac{iE}{\hbar}t}$$

where we ignore a the proportionality constant since the total solution is $\Psi(x,t)$, so we can just figure out the proportionality constant when solving for $\psi(x)$, which is typically the part most relevant for normalization. For the rest of this exam, however, we will focus on the time-independent Schrodinger equation, which is Equation (9). It is spatial portion of the wavefunction, $\psi(x)$, for which we have to be more concerned with the precise problem setup.

There's a reason that the chosen constant is denoted as E. In classical mechanics, there is a term called the **Hamiltonian** of a system, which gives the total energy of the system as the sum of its *kinetic energy* (often denoted with T) and its *potential energy* (denoted with V):

$$H = T + V$$

Since the kinetic energy is given by

$$T = \frac{p^2}{2m}$$

this gives us the classical mechanical Hamiltonian

$$H = \frac{p^2}{2m} + V \tag{10}$$

I.2.1 Exercise

Use the definition of the $\hat{p}$ operator given in Equation (4) to demonstrate that Equation (10) becomes

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$$

This allows us to write Equation (9) as

$$\hat{H}\psi(x) = E\psi(x)$$

which explains why we referred to our arbitrary constant E as the energy of the state.

II Square Wells

II.1 The Infinite Square Well

An **infinite square well** is a system where the potential energy is given by

$$V(x) = \begin{cases} 0 & 0 \le x \le a \\ \infty & x > a,\ \ x < 0 \end{cases} \tag{11}$$

In order for the energy to not blow up outside of the region $0 \le x \le a$, we must have $\psi(x) = 0$ for $x > a$ & $x < 0$. Thus, we are only concerned with the wavefunction and energies inside the well, which has a width a and spans from $x = 0$ to $x = a$.

We can rewrite Equation (9) as

$$\frac{d^2\psi}{dx^2} = -k^2\psi \text{ where } k \equiv \frac{\sqrt{2mE}}{\hbar} \tag{12}$$

where we can assume that $E \geq 0$ because $V = 0$ and we must have $E \geq V$ to avoid issues related to normalizing the wavefunction. This is the classical simple harmonic oscillator equation. Its general solution must take the form

$$\psi(x) = A\sin(kx) + B\cos(kx) \tag{13}$$

Because we established that we must have $\psi(x) = 0$ for $x < 0$ and $x > a$, and because the wavefunction must be continuous, this requires that

$$\psi(0) = \psi(a) = 0 \tag{14}$$

II.1.1 Exercise

1. Sketch the potential of the infinite square well system (i.e. sketch $V(x)$ vs. x from Equation (11))
2. Plug Equation (13) back into Equation (12) to show that the equality in Equation (12) is actually satisfied with Equation (13).
3. Using the boundary conditions given in Equation (14), show that

   $$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

   and

   $$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

   where $n \in \mathbb{N}$ (i.e. n is a natural number, with $n = 1, 2.3, ...$).

   Hint: $\sin(\pm n\pi) = 0$ and $\cos(\pm n\pi) = \pm 1$.
4. Briefly explain why n must start at 1 and not 0.
5. Let's pretend that we can get a quantum emitter to emit light at a particular wavelength λ by constructing an object with the infinite square well potential given in Equation (11) and exploiting the $n = 1$ to $n = 2$ transition of an electron (so that $m = m_e$). Basically, when an electron relaxes down from a higher-energy eigenstate (larger n) to a lower-energy eigenstate (smaller n), it can release that extra energy in the form of a photon. This is what happens in light-emitting devices such as lasers and LEDs.

   If we want this emitter to emit green light (500 nm), then what should the radius a be? Show your calculations and work. How does this compare to the radius of an atom, which is around $2 * 10^{-10}$ m (2 Å)? While this is a very crude model, this illustrates a way you can begin to think about what quantum dots are and how quantum dots work.

II.2 The Finite Square Well

Now, let us shrink the potential barrier and look at an object with the potential

$$V(x) = \begin{cases} -V_0 & |x| \leq a \\ 0 & |x| > a \end{cases} \tag{15}$$

where V_0 is a positive constant. Note that here, the width of the well is $2a$, not a, since the well potential goes from $x = -a$ to $x = +a$. Here, because of the potential setup, we can have

solutions with $E < 0$ (**bound states**) and $E \geq 0$ (**scattering states**). We will focus on the bound states for the purposes of laser emission.

In $|x| > a$, the potential is $V(x) = 0$, so Equation (9) becomes

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi \text{ where } \kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \tag{16}$$

κ is real and positive. The solution for this equation takes the general form

$$\psi(x) = Ae^{\kappa x} + Be^{-\kappa x}, \;\; |x| > a \tag{17}$$

In the region $|x| \leq a$, with $V(x) = -V_0$, Equation (9) becomes

$$\frac{d^2\psi}{dx^2} = -l^2\psi \text{ where } l \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar} \tag{18}$$

The general solution for this equation takes the form

$$\psi(x) = C\sin(lx) + D\cos(lx), \;\; |x| \leq a \tag{19}$$

When solving this system, we can save time by noting that since the potential is an even function, we can assume with no loss of generality that solutions are either even or odd, which lets us impose boundary conditions for only one side (eg. $x = a$). We encourage you to look into the proof of this claim for your own understanding, but we will not ask you to prove this here.

II.2.1 Exercise

Let's start with looking at the even solutions (where $\psi(-x) = \psi(x)$).

1. Show, by plugging in the general solution forms Equations (17) and (19) into Equations (16) and (18) for the respective ranges of x, that the wavefunction must take the form

$$\psi(x) = \begin{cases} Be^{-\kappa x} & x > a \\ D\cos(lx) & |x| \leq a \\ Be^{\kappa x} & x < -a \end{cases}$$

   In doing so, address:

   - Why the boundary conditions and evenness dictate that $\psi(x) \propto e^{-\kappa x}$ for $x > a$ and $\psi(x) \propto e^{\kappa x}$ for $x < -a$
   - Why the evenness of the wavefunction requires $\psi(x) \propto \cos(lx)$ for $|x| \leq a$

2. Use the continuity of $\psi(x)$ and $d\psi/dx$ between the different regions, at boundary points $x = \pm a$, to demonstrate that we must require

$$\kappa = l\tan(la)$$

   Hint: as noted before, the evenness of this wavefunction lets us save time by only needing to apply the boundary condition to either $x = a$ *or* $x = -a$.

3. Make the substitutions

$$z \equiv la \text{ and } z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}$$

   and use the definitions of κ and l from Equations (16) and (18) to demonstrate that the equation in the previous part gives us the condition

$$\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

   This equation has z on both sides, but it can be solved numerically by plotting both sides and finding the points of intersection.

4. Examine the following two limiting cases:

   - **Wide, deep well**
   - **Shallow, narrow well**

   Consider the following questions:

   - What happens to z_0 in each of those cases (i.e. what limiting values does it approach)?
   - What are the limiting values of z (z_n) where the intersections between $\tan z_n$ and $\sqrt{(z_0/z_n)^2 - 1}$ occur?

     What is the limit of E_n for the wide, deep well with these limiting z_n? Specify if n is even or odd, if needed.

     Hint: use the definitions of z, z_0, and l.
   - What does this limit of E_n in the case of the wide, deep well remind you of?
   - Is it possible to have zero bound states in the shallow, narrow well for the odd case, if the well is shallow and narrow enough? If it is, then what is the corresponding condition on V_0 for this to be true? If not, what is the minimum number of bound states a well must have?

II.2.2 Exercise

Now let's look at the odd solutions (where $\psi(-x) = -\psi(x)$).

1. Show, by plugging in the general solution forms Equations (17) and (19) into Equations (16) and (18) for the respective ranges of x, that the wavefunction must take the form

$$\psi(x) = \begin{cases} Be^{-\kappa x} & x > a \\ D\sin(lx) & |x| \leq a \\ -Be^{\kappa x} & x < -a \end{cases}$$

   In doing so, address:

   - Why the boundary conditions and oddness dictate that $\psi(x) \propto e^{-\kappa x}$ for $x > a$ and $\psi(x) \propto -e^{\kappa x}$ for $x < -a$
   - Why the oddness of the wavefunction requires $\psi(x) \propto \sin(lx)$ for $|x| \leq a$

2. Use the continuity of $\psi(x)$ and $d\psi/dx$ between the different regions, at boundary points $x = \pm a$, to demonstrate that we must require

$$\kappa = -l\cot(la)$$

   Hint: as noted before, the oddness of this wavefunction lets us save time by only needing to apply the boundary condition to either $x = a$ *or* $x = -a$.

3. Make the substitutions

$$z \equiv la \text{ and } z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}$$

   and use the definitions of κ and l from Equations (16) and (18) to demonstrate that the equation in the previous part gives us the condition

$$\cot z = -\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

   This equation has z on both sides, but it can be solved numerically by plotting both sides and finding the points of intersection.

4. Examine the following two limiting cases:

   - **Wide, deep well**
   - **Shallow, narrow well**

   Consider the following questions:

   - What happens to z_0 in each of those cases (i.e. what limiting values does it approach)?
   - What are the limiting values of z (z_n) where the intersections between $\cot z_n$ and $-\sqrt{(z_0/z_n)^2 - 1}$ occur?

     What is the limit of E_n for the wide, deep well with these limiting z_n? Specify if n is even or odd, if needed.

     Hint: use the definitions of z, z_0, and l.
   - What does this limit of E_n in the case of the wide, deep well remind you of?
   - Is it possible to have zero bound states in the shallow, narrow well for the odd case, if the well is shallow and narrow enough? If it is, then what is the corresponding condition on V_0 for this to be true? If not, what is the minimum number of bound states a well must have?

II.2.3 Question

Compare and contrast $\psi(x)$ outside of the well (eg. for $x > a$) in the finite and infinite well cases. Provide your interpretation of what this means for a particle starting inside the well and whether it can ever leave the well in each of those cases. Also compare each case to what we expect in classical mechanics. This relates to the phenomenon known as **quantum tunneling**.

III Quantum Cascade Laser Design

III.1 Single-Well Design

If our design were to consist of a single well, it would look exactly like the finite-well problem. Below is a graph of the potentials and the first two eigenstates of the single finite well problem:

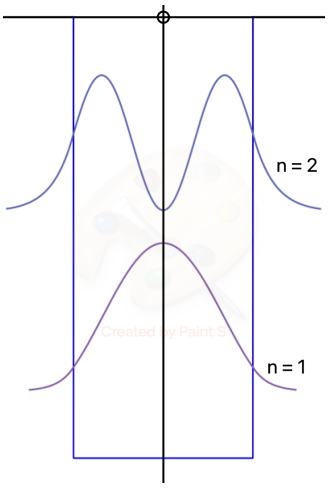

Figure 1: Sketch of a single finite well with the "$n = 1$" and "$n = 2$" eigenstates

Here you see sketches of the *square of the wavefunctions* for the first two bound eigenstates in the well, corresponding to the lowest two values of z such that the boundary condition criteria

were satisfied for the even or odd solutions of $\psi(x)$. Be careful, because while the well is plotted as energy E versus x, the wavefunction is plotted as $|\psi(x)|^2$ vs. x. You can also think back to the infinite well, when $E_n \propto n^2$ for natural numbers n, although the exact wavefunctions and energy values are different for this finite-well case.

In practice, these quantum wells are made by alternating materials, generally *semiconductors*, with different band gaps. Check out this link (`https://energyeducation.ca/encyclopedia/Band_gap`) for more information about metals vs. semiconductors vs. insulators, conduction and valence bands, band gaps, etc. Suffice it to say, conduction bands are the lowest "unoccupied" energy level in a material in which electrons are allowed (I use quotes because random thermal excitations of electrons means that there is always a miniscule number of electrons in the conduction band for temperatures above 0K, but it's still a tiny fraction of the total electron number. In common semiconductors, this fraction is anywhere from 10^{-12} to 10^{-16} at room temperature).

The sketch in Figure 1 is inspired by the author's research on gallium arsenide (GaAs)-based quantum cascade lasers. It shows the conduction bands of GaAs and aluminum gallium arsenide (AlGaAs). The middle region, with $|x| < a$, is made of GaAs, and it is surrounded to the left and right by layers of AlGaAs, which has a higher band gap. The composition of AlGaAs can vary by changing the relative fractions of aluminum (Al) and gallium (Ga). Technically, its composition must be expressed as $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$.

When $x = 1$, we have pure aluminum arsenide (AlAs), with a band gap of 2.16 eV (and gives rise to the maximum possible finite barrier height) while with $x = 0$ we have pure GaAs and there is no barrier height and therefore no well. For compositions in-between, if we focus on the position of the conduction band (which we will call E_C) we can estimate it as

$$E_C(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}) = xE_C(\mathrm{AlAs}) + \big(1-x\big)E_C(\mathrm{GaAs}) \tag{20}$$

When designing a quantum well, we saw earlier that the intersection values z in the finite-well solution depended on z_0, which was defined in terms of both a, (half of) the well width, and V_0, the well depth, so both V_0 and a dictate the energy levels and can help achieve the desired emission wavelenegth. In practice, you would start with setting V_0 by tuning the composition of the heterostructure (in this case, by adjusting x in $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$). This is because when semiconductors have different lattice constants (distance between the closest repeating units in a crystal, such as the difference between the nearest sodium atoms in a sodium chloride crystal) growing them on top of each other introduces **lattice strain** because of this difference, stretching or compressing the crystal, which introduces unwanted defects and makes device performance suffer.

Because of this, we want x to be as small as possible so that the lattice constants are as similar between the two materials as possible, which will let us minimize lattice strain and its associated defects. On the other hand, we also want our well to be tall enough to contain the desired number of energy states (no fewer than two, but needing at least three in practice). Therefore, by optimizing the composition to balance these two constraints, we can set our V_0, and from there we can use the finite-well expressions to solve for a well width $2a$ that will obtain the desired energy offsets between adjacent energy levels. This gives us a way to solve the conundrum of "V_0 or a first?": first optimize V_0 for lattice strain and energy state confinement, then set a to obtain the desired emission energy.

III.1.1 Question

1. Draw Figure 1 for yourself (either by hand or on the computer). Based on the sketches of the squares of the wavefunctions for the first two bound eigenstates, clearly indicate where a particle in the $n = 1$ state is most likely to be. Do the same for a particle in the $n = 2$ state.

2. Can a particle that starts off inside the well find itself outside of the well? Why or why not? If it can, draw vertical dotted lines in your figure to indicate the maximum distance to the left and right of the y axis that the particle can travel / exist. If it cannot, you do not need to do anything more.

3. What does the previous part tell us about the possibility of quantum tunneling? If quantum tunneling can occur, what does the previous part tell us about the placement of adjacent finite quantum wells to the left and right of this one in order to permit tunneling from one well to another?

III.1.2 Exercise

Let us say that the conduction band offset between the conduction bands of GaAs and AlAs is 230 meV (milli-electron volts) (in reality, there is a non-linearity, but to simplify, we will assume that in this problem the maximum conduction band offset occurs for an $x = 1$ $Al_xGa_{1-x}As$ alloy composition).

Suppose you run some simulations and determine that you need a band offset of 189 meV to minimize lattice strain while sufficiently containing the $n = 1$ and $n = 2$ eigenstates so that you have at least two bound states to allow emission to occur. What is the concentration of aluminum (value of x) in $Al_xGa_{1-x}As$ that will yield the desired band offset?

III.1.3 Question

Because of the non-zero aluminum content found in the previous exercise, the resulting quantum well structure will exhibit lattice strain, which will alter the results from what we expect with our current model. Let us say that the strain stretches the well, such that the width of the well is *wider* than what we expect when providing the crystal growers with the growth parameters and layer thicknesses.

1. Will this affect the individual energy levels? If so, then how?

2. Will this affect the spacing between energy levels? IF so, then how?

III.2 Two-Well System

Below is the sketch of two finite-barrier quantum wells connected by a thin barrier to permit quantum tunneling between the wells:

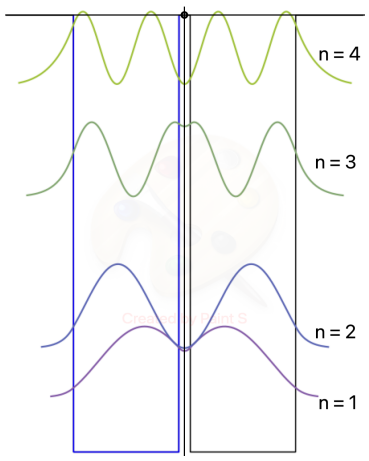

Figure 2: Sketch of the squares of the wavefunctions for different energy levels in a two-well system. The origin of the system is indicated by the intersection of the x and y axes and marked by the black dot.

Since the well heights are the same as in the one-well case, we see that the $n = 1$ and $n = 2$

energy states in the one-well case have now split into two states each. Now, we are concerned with the transition between the new $n = 3$ and $n = 2$ states for photon emission. The transition between the new $n = 2$ and $n = 1$ states, on the other hand, tends to result in the emission of phonons (lattice vibrations, so basically quantized sound waves) for reasons we will not get into here. This will be true from here on out, so we will concern ourselves mostly with the transition between the $n = 2$ and $n = 3$ states.

III.2.1 Question

1. Comment on the shape of the wavefunctions of the new $n = 1$, $n = 2$, $n = 3$, and $n = 4$ states in this two-well system and compare them to the old $n = 1$ and $n = 2$ states in the one-well system. Focus on the portion of the new wavefunctions in one of these wells (eg. the right well).
2. What does this tell you about the splitting of the states when going from the old one-well case to the new two-well case? Specifically, the old $n = 1$ corresponds to which of the n state(s) in the new well? What about the old $n = 2$ state − which of the n states in the new well does it correspond to?

III.2.2 Exercise

Following the setup of the single finite well and in accordance with the sketch in Figure 2, set up the two-well problem. To help you, I will give you the potential of the system shown in Figure 2:

$$V(x) = \begin{cases} 0 & |x| < b/2, \;\; |x| > b/2 + a \\ -V_0 & b/2 \leq |x| \leq b/2 + a \end{cases}$$

where a is the width of the well and b is the width of the barrier coupling the two wells.

Is the potential even or odd (or neither)? What does that tell us about the form of the wavefunction? If the wavefunction must be even or odd, you can choose to focus on the odd wavfunction case. Your wavefunction should be written as a piecewise function, similar to the one-well finite barrier case in an earlier section, that takes the form

$$\psi(x) = \begin{cases} f(x) & x > b/2 + a \\ g(x) & b/2 \leq x \leq b/2 + a \\ h(x) & |x| < b/2 \\ j(x) & -b/2 - a \leq x \leq -b/2 \\ q(x) & x < -b/2 - a \end{cases}$$

where $f(x)$, $g(x)$, $h(x)$, $j(x)$, and $q(x)$ are various functions of x that may or may not be related to each other.

What are the relevant boundary conditions, and what constraints do they give us? Try to follow the general steps in the finite square well exercises as closely as possible, although your expressions will be different in this exercise because the potential is different.

III.2.3 Question

1. Based on what you know about the wavefunction of a state inside and outside a finite square well, should you make your barriers between your wells thicker or thinner in order to maximize tunneling between wells?
2. Growing single atomic layers is a difficult and time-consuming process. As a result, material growers prefer to have layers at least three atomic layers thick ($\sim$ 3-9 Å). Does this create a trade-off between tunneling and minimum well thickness?

III.3 Three-Well System

Many quantum cascade lasers use at least three quantum wells in a single active region unit because it allows for both vertical and diagonal transitions when a potential bias is applied to the system (which we will explore later). Below is a diagram illustrating such a three-well system:

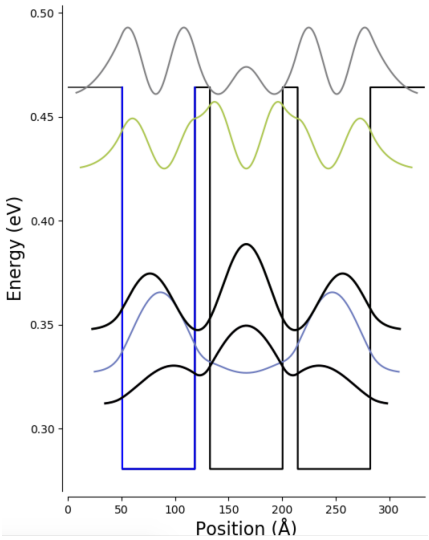

Figure 3: Diagram of a three quantum well active region.

The more overlap between the wavefunctions of each state, the better the tunneling will be between them because the more likely that being at a given electron energy will mean being able to move back and forth easily between the overlapping states. Therefore, the narrower the spread in wavefunctions arising from the splitting of a given one-well band, the better the electron transport through the system.

III.3.1 Question

1. What do the shapes and positions of the wavefunctions parallel to the energy axis tell you about the splitting of the old, one-well $n = 1$ and $n = 2$ energy levels into the levels seen in this three-well system?
2. How many of the energy levels pictured in Figure 3 correspond to the old one-well $n = 1$ state? How many of the ones pictured here correspond to the old $n = 2$ state? Redraw Figure 3 and indicate on your drawing which ones correspond to each.
3. Are your responses to the previous part the same for the old $n = 1$ and old $n = 2$ states? Is this what you would expect based on our discussion of the two-well system? If not, what do you think is the reason for this discrepancy? What is the implication of this for a particle in an excited state in this system? Will the particle be more or less likely to stay within the wells compared to the one-well and two-well cases discussed earlier?

III.3.2 Question

What do you think will happen if more wells are added to the system, assuming the same well and coupling barrier widths?

III.4 Biased Three-Well Active Region

Biasing the structure by applying a voltage to it puts the first quantum well at at a higher potential than the last one and tilts all the well bottoms and barriers themselves. Because the

energy levels all started out flat, applying a constant voltage to the system will tilt the entire system the same. Below is a diagram of a biased three-well system where all the well widths are the same thickness a and all the coupling barriers are the same thickness b when the system is unbiased:

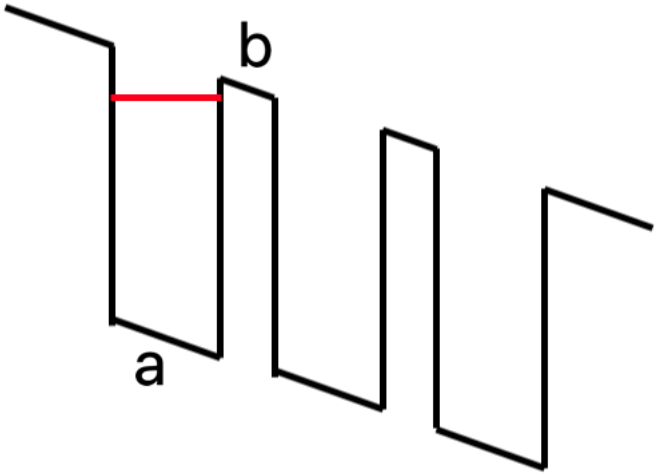

Figure 4: Sketch of a biased three-well system with each well having width a and each coupling barrier having width b. The red line pictured is for the purposes of one of the questions in this section.

The red line in Figure 4 is for the purposes of one of the questions in this section.

III.4.1 Exercise

Write an expression for the potential $V(x)$ of the system using the fact that each well width is a and each barrier width is b (but note that the "barriers" at the left and right edges extend out to $\pm\infty$). You can call the slope of the potential c. Your potential expression will be a piecewise function, as we have seen before for all the other quantum well systems.

III.4.2 Question

These diagrams, which show quantum wells made of conduction bands, plot the energy of an electron, which is a negatively charged particle. Thus, in Figure 3, an electron in the lower energy states will have an electron energy that's 0.3-0.4 eV above the bottom of the well.

Based on this, how is the system biased? In other words, to which side will you apply the positive voltage and to which side will you apply the negative voltage? Sketch Figure 4 and label the + and - terminals in the figure.

III.4.3 Question

1. Compare the alignment of the wells in the biased system shown in Figure 4 to that of the unbiased system shown in Figure 3. What does this tell you about the alignment of the energy levels if we look at each well in the system separately (i.e. pretend that they are uncoupled and much further apart)?

2. Based on your answer to the previous part, will you achieve the best energy band alignment (and therefore the narrowest spread in the wavefunctions) by making all three wells the same width? Use your answer to the previous part to support your claim. If the wells should be of different widths, then sketch a biased three-well system and indicate the relative widths of each of the wells (i.e. which one is the widest, which is the narrowest, and which is in the middle, thickness-wise).

Hint: you can refer back to the expression for energy levels in the infinite-well system, which most explicitly gives the relationship between energy levels and well thickness. Even though this is not an infinite well system, the qualitative behavior follows a roughly similar relationship.

III.4.4 Question

1. Now let's think specifically about the excited states in this system. Consider an excited state inside the left-most well, but near the top of this well, as shown by the red line in Figure 4. Remember, the energy of a *given* state is the same throughout the system at all positions.

   Based on this, where will the wavefunction of this state be relative to the tops of the middle and right-most well? What does this tell you about whether an electron in this state will be contained inside these wells if tunneling occurs? Can this cause problems in the operation of this device? If so, what problems?

2. Below is a figure of the same three-well system, but this time it is at a higher bias:

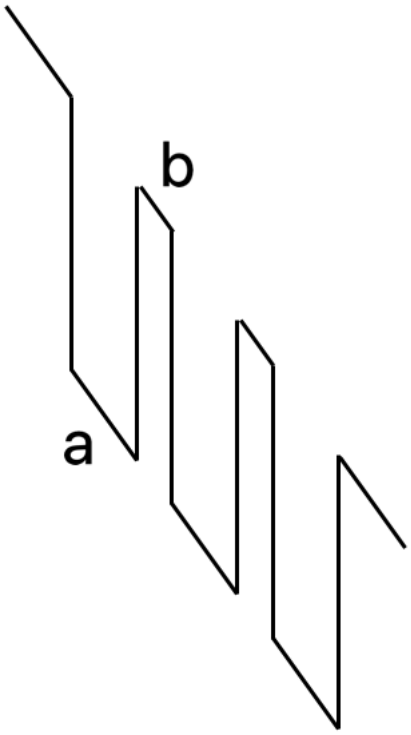

Figure 5: Three-well system at a higher bias than before

   How will this higher bias affect tunneling through the barriers? Why is that? Use the geometry of the situation and the fact that the unbiased well and barrier widths, a and b respectively, are still the same in this system as compared to Figure 4. How will this affect electron transport through the device?

3. Based on your answers to the previous parts of this question, is there a trade-off to consider when deciding on the appropriate bias to apply to the system? If so, what is this trade-off?

III.5 Full Quantum Cascade Laser System (Active + Injector Region)

Finally, we will look at the "full" quantum cascade laser system unit, which will contain two active regions bridged by an injector region. A full laser will have millions of such units, but

they will simply repeat this unit, so examining this will tell us everything we need to know about the core physics of this system and its emission. Below is a diagram of this system:

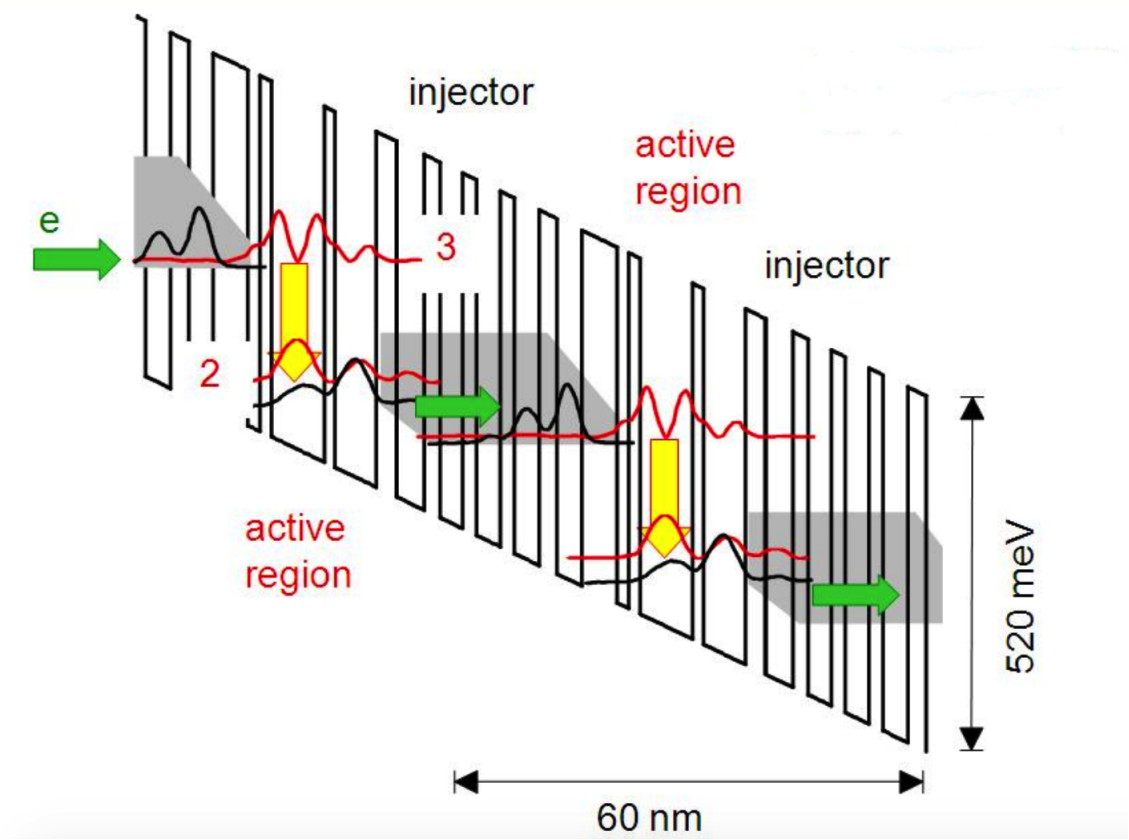

Figure 6: Schematic of two active regions bridged by an injector region, with an injector region to the left of the left active region and right of the right active region as well.

III.5.1 Question

1. Based on the schematic in Figure 6 and everything you have learned about quantum wells and quantum cascade lasers, explain how a quantum cascade laser works. Remember that an electron can drop down to a lower-energy state and emit a photon in the process. Start with an electron entering through the injector region on the left and trace its path through the device as sketched above. Use the arrows to help guide you and describe what is happening at each of these stages labeled by said arrows.

2. What is the purpose of the injector region? What must you try to achieve (specifically with the alignment of different energy states) in order to accomplish this goal? Based on this, is there more flexibility or less when setting the widths of the wells in the injector regions as compared to those of the active regions?

3. In order for a laser to lase and emit light at its high power (higher than LEDs and other light sources we commonly use), it must achieve ***gain***, which (in this context) is when the energy of the surroundings (in this case, coming from the potential bias of the system) can be used to amplify the emission, such that a single electron can emit multiple photons.

   Explain, with the help of the schematic in Figure 6, how the biased quantum well structure in this quantum cascade laser can give rise to such laser gain. Do you understand why it is called a quantum *cascade* laser now? Can you explain why this is so?

III.5.2 Question

Summarize the parameters that we have discussed that are relevant to laser design as well as all trade-offs that we have discussed (and any others that you may be able to come up with)!

IV Afterword

Congratulations on making it to the end of this assignment! If you have gone through all the sections and engaged with the questions and exercises, you should now have a solid understanding of the basics of quantum cascade laser physics, how this laser works, and the design parameters, principles, and limitations that need to be considered when designing one of these devices. We hope you enjoyed the exam, that you learned a lot, and that this may have sparked an interest in learning more!