2021 PUEC Solutions - Team Spherical Humans (Notes)

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March 2021

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The Schrodinger Equation tells us

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

$$\implies \frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi$$

Upon taking the complex conjugate, it is then seen that

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

$$\implies \frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*$$

Using the product rule, we see that

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi$$

We can use the Schrodinger equation to substitute into this expression:

$$= \Psi^*\left(\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi\right) + \Psi\left(-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*\right)$$

$$= \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \Psi\frac{\partial^2\Psi^*}{\partial x^2}\right) - \frac{i}{\hbar}(\Psi^*V\Psi - \Psi V\Psi^*)$$

The potential is observable and hence a Hermitian operator, which shows that the expectation must be real-valued, since $(\Psi^* V \Psi)^\dagger = \Psi^* V^\dagger \Psi$. Taking complex conjugates, we can show that $\Psi^* V \Psi = (\Psi^* V \Psi)^* = \Psi V^* \Psi^* = \Psi V \Psi^*$. Hence, the potential expectations are equal and cancel out. From the product rule again, we can write that

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)$$

We can substitute this result into the given equation to show that

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

Pulling out the constant, we conclude that

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

This completes part 1 of the exercise. Using the result of part 1, we can see that the expectation value $\langle \hat{p} \rangle$ would follow

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

Note that this is slightly different than the form given in the text, which drops the m. Now to continue, we must use integration by parts. Note that for two functions f and g, it can be written that

$$\int_a^b f\frac{\partial g}{\partial x}\,\mathrm{d}x = fg\Big|_a^b - \int_a^b \frac{\partial f}{\partial x} g\,\mathrm{d}x$$

Identifying $f(x,t) = x$ and $g(x,t) = \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi$, and taking the bounds of integration from $-\infty$ to ∞, we see that

$$\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\mathrm{d}x = \left[x\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\right|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\mathrm{d}x$$

If we demand our wavefunction is normalizable and vanishes at infinity, the evaluation term vanishes. Putting back in constant factors, we are left with

$$\langle \hat{p} \rangle = \frac{i\hbar}{2}\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\mathrm{d}x = -\frac{i\hbar}{2}\int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\mathrm{d}x$$

Note that $\left(\Psi^* \frac{\partial \Psi}{\partial x}\right)* = \frac{\partial \Psi^*}{\partial x}\Psi$. Also, note that $\frac{1}{2}(z - z*) = \mathrm{Im}\{z\}$. Thus, we can rewrite the integral as

$$= -i\hbar\int_{-\infty}^{\infty}\mathrm{Im}\left\{\Psi^*\frac{\partial \Psi}{\partial x}\right\}\mathrm{d}x = -i\hbar\,\mathrm{Im}\left\{\int_{-\infty}^{\infty}\Psi^*\frac{\partial \Psi}{\partial x}\,\mathrm{d}x\right\}$$

Note that since momentum is an observable and hence a Hermitian operator ($\hat{p} = \hat{p}^\dagger$), its imaginary part must be zero, so its expectation must be real-valued. This means that the integral must evaluate to a pure imaginary number. Bringing in constants, we can get rid of the Im and rewrite the integral as

$$= \int_{-\infty}^{\infty}\Psi^*\left(-i\hbar\frac{\partial \Psi}{\partial x}\right)\mathrm{d}x$$

In summary, we have shown that

$$\langle \hat{p} \rangle = m\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t} = \frac{i\hbar}{2}\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\Psi^*(x,t)\frac{\partial \Psi(x,t)}{\partial x} - \frac{\partial \Psi^*(x,t)}{\partial x}\Psi(x,t)\right)\mathrm{d}x = \int_{-\infty}^{\infty}\Psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x,t)\,\mathrm{d}x$$

This leads us to conclude that the form of the momentum operator should be

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

I.1.2 Exercise

Expanding we have

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

By linearity of expectation, we can pull out the terms, and

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

And since $\langle j\rangle$ is constant, the average of $j\langle j\rangle$ is simply $\langle j\rangle\langle j\rangle = \langle j\rangle^2$. Plugging this in we get the desired

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

I.1.3 Exercise

1. We need

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 \,\mathrm{d}x = \int_0^a A^2 \sin^2\left(\frac{\pi x}{a}\right) \mathrm{d}x = 1$$

The average value of $\sin^2$ is $1/2$, and the given bounds perfectly covers one period of $\sin^2$, so the integral is simply

$$\int_0^a A^2 \sin^2\left(\frac{\pi x}{a}\right) \mathrm{d}x = \frac{A^2 a}{2}$$

Thus, $A = \sqrt{\frac{2}{a}}$.

2. By definition

$$\langle \hat{x}\rangle = \int_{-\infty}^{\infty} x\Psi(x)^2 \,\mathrm{d}x = \frac{2}{a}\int_0^a x\sin^2\left(\frac{\pi x}{a}\right)\,\mathrm{d}x.$$

However, we do not need to actually compute this integral. Note that everything is symmetric about $a/2$, and thus $\langle \hat{x}\rangle = a/2$. Similarly for momentum, using the equation given,

$$\langle p\rangle = -i\hbar\int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\frac{\partial\Psi(x)}{\partial x}\,\mathrm{d}x = -\frac{i\hbar}{a}\int_0^a 2\sin(\pi x/a)\cos(\pi x/a)\,\mathrm{d}x.$$

Applying the double angle formula, the integrand becomes $\sin\left(\frac{2\pi x}{a}\right)$. Since the integration covers the full period of the sine function, we get

$$\langle p\rangle = 0.$$

3. First for x using equation (6),

$$\sigma_x^2 = \int_{-\infty}^{\infty} x^2\psi(x)^2\,\mathrm{d}x - (a/2)^2.$$

We can write the first integral as

$$\frac{2}{a}\int_0^a x^2\sin^2\left(\frac{\pi x}{a}\right)\,\mathrm{d}x$$

Using the substitution $\sin^2(\pi x/a) = (1-\cos(2\pi x/a))/2$ and integrating by parts twice, we obtain

$$\sigma_x^2 = a^2\left(\frac{1}{3} - \frac{1}{2\pi^2}\right)$$

For p, using equation (7),

$$\sigma_p^2 = \int_{-\infty}^{\infty}\Psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)^2\Psi(x,t)\,\mathrm{d}x - 0^2 = -\hbar^2\int_0^a -\frac{2}{a}\frac{\pi^2}{a^2}\sin^2\left(\frac{\pi x}{a}\right)\,\mathrm{d}x = \frac{\pi^2\hbar^2}{a^2}.$$

So we can check that

$$\sigma_x\sigma_p = a\sqrt{\frac{1}{3} - \frac{1}{2\pi^2}}\frac{\hbar\pi}{a} = \hbar\sqrt{\frac{\pi^2}{3} - \frac{1}{2}} \approx 1.670\hbar \geq \hbar/2.$$

I.2 Separation of Variables

I.2.1 Exercise

Equation 4 tells us that $\hat{p} = -i\hbar\frac{\partial}{\partial x}$. Thus,

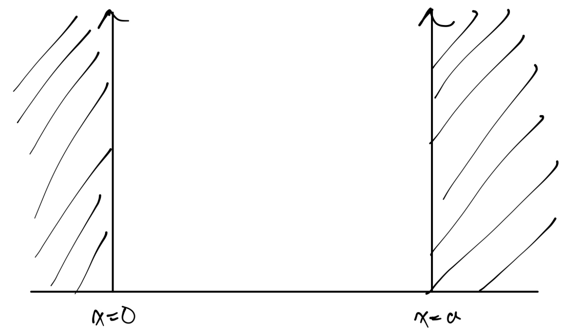
$$\hat{H} = \frac{\hat{p} \cdot \hat{p}}{2m} + V = \frac{\hat{p}^2}{2m} + V = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V.$$

II Square Wells

II.1 The Infinite Square Well

II.1.1 Exercise

1. The potential will follow the graph as shown below



2. We know that
$$\psi(x) = A\sin(kx) + B\cos(kx).$$
To show that this co-aligns with equation 12, we must calculate both sides and see if they equate to this general form. Note that
$$\frac{d\psi}{dx} = -k(B\sin(kx) - A\cos(kx)) \implies \frac{d^2\psi}{dx^2} = -k^2(A\sin(kx) + B\cos(kx)).$$
Hence, this form is the same as $-k^2\psi$ meaning that this general form of ψ satisfies equation 13.

3. Boundary conditions require that $\psi(0) = \psi(a) = 0$. For $\psi(0)$ specifically, we know that
$$\psi(0) = A\sin(0) + B\cos(0) = B \implies B = 0.$$
Hence, $\psi(x) = A\sin(kx)$. We also know that for $\psi(a)$,
$$\psi(a) = A\sin(ka) \implies A = 0, \text{ or } \sin(ka) = 0.$$
It is trivial when $A = 0$ since we are left with only a nonnormalizable solution of $\psi(0) = 0$. This means that we must take the other option of $\sin(ka) = 0$. As per the hint, $\sin(\pm n\pi) = 0 \; \forall n \in \mathbb{N}$ which means that $ka = n\pi \implies k = \frac{n\pi}{a}$. All possible values of E_n then follow
$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}.$$
We normalize $\psi(a)$ to find the value of the constant A. Note that
$$\int_0^a \psi(a)^2 \, dx = \int_0^a (A\sin(kx))^2 \, dx = \frac{A^2 a}{2} = 1 \implies A = \sqrt{\frac{2}{a}}.$$
Hence all solutions of $\psi_n(x)$ are then
$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right).$$

4. As seen in part 3, we find that solutions are trivial for $k = 0$ since there will be non-normalizable solutions of $\psi(x) = 0$, and since $\sin(x)$ is an odd function, all negative numbers are the same as positive ones and will be "absorbed" in the solution.

5. The quantum emitter in this case will essentially be emitting light through the changing from the n-th energy level to the $(n-1)$th energy level. Specifically in this problem, we are looking at the $n=1$ to $n=2$ transfer. Hence, we can write
$$\Delta E = E_2 - E_1 = \frac{3\pi^2\hbar^2}{2ma^2}.$$
We equate this to the energy of a photon or $2\pi\hbar c/\lambda$ to obtain
$$\frac{2\pi\hbar c}{\lambda} = \frac{3\pi^2\hbar^2}{2ma^2} \implies a = \sqrt{\frac{3\pi\hbar\lambda}{4mc}}.$$
Plugging in numbers with
$$\begin{aligned} \lambda &= 5.00 \times 10^{-7}\ \text{m} \\ m = m_e &= 9.11 \times 10^{-31}\ \text{kg} \\ \hbar = \frac{h}{2\pi} &= 1.05 \times 10^{-34}\ \text{J} \cdot \text{s} \\ c &= 3.00 \times 10^{8}\ \text{m/s} \end{aligned}$$
which gives us approximately $a \approx 6.74 \times 10^{-10}$ m $= 6.74$Å. This is on the order of the size of an atom, larger than the prescribed value in the text by a factor of roughly 3.

II.2 The Finite Square Well

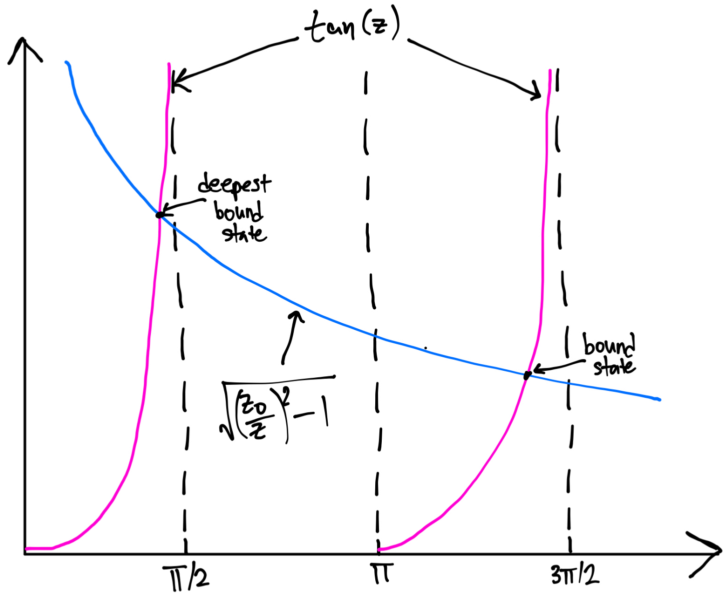
II.2.1 Exercise

1. Let us consider each region individually. We know that for the region $|x| > a$, the general solution takes the form of
$$\psi(x) = Ae^{\kappa x} + Be^{-\kappa x}, \ \ |x| > a.$$
Now consider the region $x > a$. By demanding the wavefunction is normalizable, the wavefunction must vanish as $x \to \infty$. Hence, in this region, $A = 0$ to guarantee $\lim_{x\to\infty} \psi(x) = 0$. We are left with $\psi(x) = Be^{-\kappa x}$. Since we are considering even solutions, $\psi(-x) = \psi(x)$ by definition. For the region $x < -a$, the wavefunction solution must follow $\psi(x) = Be^{-\kappa(-x)} = Be^{\kappa x}$. We can check that $\lim_{x\to-\infty} \psi(x) = 0$. For $|x| \le a$, we have the general solution of $\psi(x) = C\sin(lx) + D\cos(lx)$ and since we are only looking for even solutions, we take the $\cos(lx)$ part since $\cos(lx)$ is even and $\sin(lx)$ is odd. Hence, our wavefunction takes the form of
$$\psi(x) = \begin{cases} Be^{-\kappa x} & x > a \\ D\cos(lx) & |x| \le a \\ Be^{\kappa x} & x < a \end{cases}.$$

2. The evenness of this wavefunction lets us save time by only needing to apply the boundary condition to either $x = a$ or $x = -a$. Therefore, let us consider the boundary at $x = a$. Since $\psi(x)$ must remain continuous, we must have
$$Be^{-\kappa a} = D\cos(la)$$
and taking $d\psi/dx$ tells us
$$-\kappa Be^{-\kappa a} = -lD\sin(la) \implies \kappa = l\tan(la)$$
upon dividing both equations.

3. Equation 16 tells us that $\kappa = \frac{\sqrt{-2mE}}{\hbar}$ and equation 18 tells us $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$ which means that $\kappa^2 + l^2 = 2mV_0/\hbar^2$. We need to make the substitutions
$$z \equiv la \text{ and } z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}$$
which can let us equivalently write that
$$(l\tan(z))^2 + l^2 = \frac{z_0^2}{a^2} \implies \tan^2(z) + 1 = \frac{z_0^2}{z^2} \implies \tan(z) = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}.$$
We take the positive root because of the following observation. Note that $\tan(z) = \kappa/l$, where κ and l are strictly positive for a bound particle. Hence, $\tan(z) > 0$, and we take the positive square root.

4. As directed, let us graph transcendental solutions by plotting both $\tan(z)$ and $\sqrt{(z_0/z)^2-1}$ to obtain the graph below



- **Wide, deep well** In a wide, deep well, since $z_0 \propto a\sqrt{V_0}$, z_0 can be made arbitrarily large. In this limit, most intersections occur slightly before the vertical asymptotes at $z_n = (2n-1)\pi/2,\ n \in \mathbb{N}$, i.e. all odd multiples of $\pi/2$. However, $z \leq z_0$ for bound particles, so:

$$(2n-1)\frac{\pi}{2} \leq \frac{a}{\hbar}\sqrt{2mV_0}$$

  This shows that the number of bound states can be made arbitrarily large. Furthermore, we can show that:

$$\frac{z}{z_0} = \frac{\hbar l}{\sqrt{2mV_0}} = \sqrt{1+\frac{E}{V_0}}$$

$$\implies E_n = V_0\left(\left(\frac{z_n}{z_0}\right)^2 - 1\right)$$

$$E_n = \frac{(2n-1)^2\pi^2\hbar^2}{2m(2a)^2} - V_0,\ n \in \mathbb{N}$$

  which is very similar to an infinite square well with width $2a$ as $V_0 \to \infty$, except shifted by V_0 since we've set the top of the well to $V = 0$ by definition. Note that we only have odd energy levels of the infinite square well because we are working with a strictly even wavefunction, which excludes half of the energy levels. Making an analogy in terms of standing waves, we only keep the odd numbered harmonics (central antinode) in this solution.

- **Shallow, narrow well** As the well is shallow, z_0 eventually approaches 0. As z_0 decreases, there will be less and less bound states. However, it is not possible to have zero bound states and when $z_0 < \pi/2$ there is only one bound state that is left. When z_0 gets very small, the bound state corresponds to very small z, so we can take the Taylor expansion of $\tan z$ around $z = 0$ to get the following equation:

$$\tan z \approx z = \sqrt{(z_0/z)^2 - 1}$$

  We get a quadratic in z^2, but since $z \ll 1$, we discard the second-order term, and get $z \approx z_0$ as the only bound state. This corresponds to an energy of $E = V_0\left(\left(\frac{z}{z_0}\right)^2 - 1\right)$ as per the derivation in the wide, deep well, so energy also approaches 0.

II.2.2 Exercise

1. We now essentially follow the same steps as the previous exercise and hence this solution will be more brief. As in the previous exercise it is apparent that the general solution for the region $|x| > a$ takes the form of

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

In $x \to \infty$, the first term increases rapidly so we must choose that $A = 0$ since $\psi(x) = 0$ for the region $x > a$. Hence, we are left with $\psi(x) = Be^{-\kappa x}$. Since we are looking for odd solutions here $\psi(-x) = -\psi(x)$, then the solution for the wavefunction $\psi(x)$ in the region $x < -a$ follows $\psi(x) = -Be^{-\kappa(-x)} = -Be^{\kappa x}$. For $|x| \leq a$, we have the general solution of $\psi(x) = D\sin(lx) + C\cos(lx)$ and since we are only looking for odd solutions, we take the $\sin(lx)$ part since $\sin(lx)$ is odd and $\cos(lx)$ is even. Hence, our wavefunction takes the form of

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

2. 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 $x = -a$. Therefore, let us consider the boundary at $x = a$. Since $\psi(x)$ must remain continuous, we must have

$$Be^{-\kappa a} = D\sin(la),$$

and taking $d\psi/dx$ tells us

$$-\kappa Be^{-\kappa a} = lD\cos(la) \implies \kappa = -l\cot(la)$$

upon dividing both equations.

3. Equation 16 tells us that $\kappa = \frac{\sqrt{-2mE}}{\hbar}$ and equation 18 tells us $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$ which means that $\kappa^2 + l^2 = 2mV_0/\hbar^2$. We need to make the substitutions

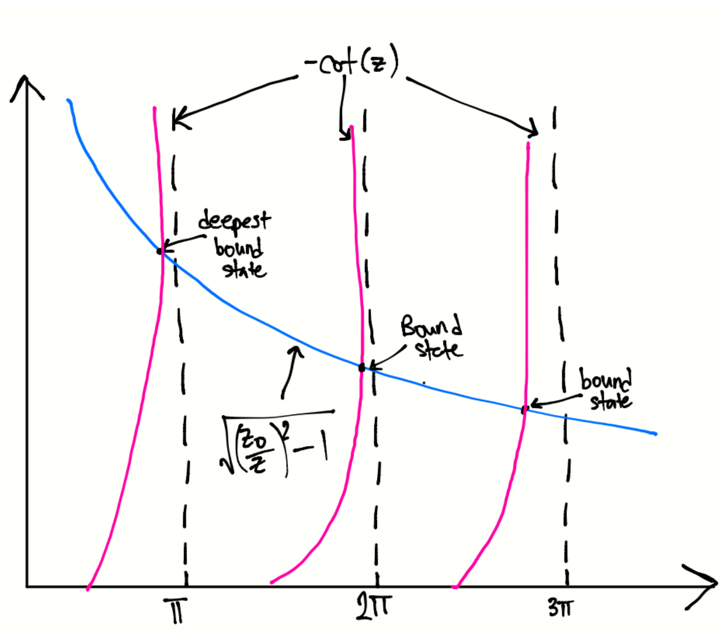
$$z \equiv la \text{ and } z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}$$

which can let us equivalently write that

$$(-l\cot(z))^2 + l^2 = \frac{z_0^2}{a^2} \implies \cot^2(z) + 1 = \frac{z_0^2}{z^2} \implies \cot(z) = -\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}.$$

We take the negative root because of the following observation. Note that $\cot(z) = -\kappa/l$, where κ and l are strictly positive for a bound particle. Hence, $\cot(z) < 0$, and we take the negative square root.

4. Let us again plot the transcendental solutions for this graph.



- **Wide, deep well** The solutions will follow the same analysis as the previous exercise except now all intersection will occur just slightly before the vertical asymptote $z_n = n\pi,\ n \in \mathbb{N}$ line. Recall that

$$E_n = V_0\left(\left(\frac{z_n}{z_0}\right)^2 - 1\right)$$

$$\implies E_n \approx \frac{(2n)^2\pi^2\hbar^2}{2m(2a)^2} - V_0,\ n \in \mathbb{N}.$$

  Like the previous solution with even wavefunctions, this gives energy levels of an infinite square well with width $2a$ as $V_0 \to \infty$, shifted by V_0 due to our definition of the top of the potential being $V = 0$. Note that these energy levels include only even energy levels of the infinite square well, since we are working with a strictly odd wavefunction, which excludes half of the energy levels. Making an analogy in terms of standing waves, we only keep the even numbered harmonics (central node) in this solution.

- **Shallow, narrow well** As in the previous exercise, z_0 approaches 0. There are no intersections below a certain value of $z_0 < \pi/2$. For $\frac{\pi}{2} \leq z_0 < \frac{3\pi}{2}$, there will be one intersection. Therefore, if the potential satisfies

$$z_0 = \frac{\sqrt{2mV_0}}{\hbar}a < \frac{\pi}{2} \implies V_0 < \frac{\pi^2\hbar^2}{2m(2a)^2}$$

  there are no possible bound states that are odd.

II.2.3 Question

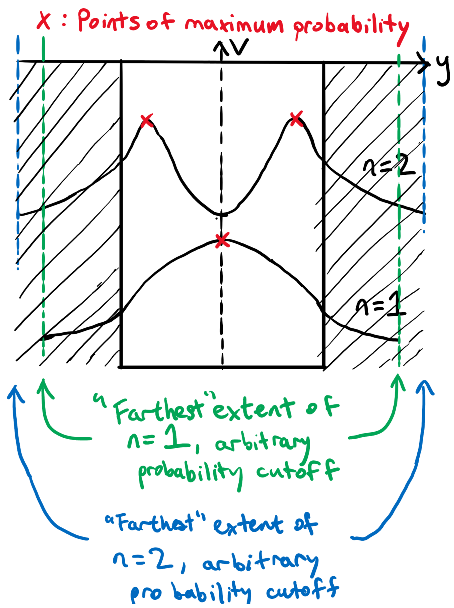
$\psi(x)$ is nonzero outside the well for a finite square well. This leads to the important result that in quantum mechanics, upon measurement, a particle can be found in a classically forbidden region, i.e. one where $E + V < 0$! In classical mechanics, this will never happen by conservation of energy, but we have shown that it happens in quantum mechanics. As the well gets deeper and approaches an infinite well, the wavefunction vanishes outside the well. This means that the deeper the well, the less likely the particle will be found in a classically forbidden region outside the well ("leave the well"), with the probability going to 0 as the well gets infinitely deep. If the particle is measured to be outside the well, we can say that it has tunnelled.

III Quantum Cascade Laser Design

III.1 Single-Well Design

III.1.1 Question

1. While the the well is plotted as E versus x, the probability density is plotted as $|\psi(x)|^2$ versus x. The $n = 1$ energy level is unimodal and the particle is likely to be in the middle of the well, while the $n = 2$ energy level is bimodal and has two symmetric locations of maximum likelihood for the position of the particle, though the expectation value of position is still in the center of the well for both.



2. Though the wavefunction (and probability amplitude) exponentially decays and never exactly reaches zero outside the well, the nature of the exponential decay means that after some distance outside the well, the probability of finding the particle is *essentially* zero. In the given figure, the wavefunctions seem to be plotted in the rough domain $|x| < 2a$, i.e. in a region twice as wide as the well.

3. Quantum tunneling is possible, though the probability of tunneling falls off exponentially with distance from the well. To ensure reliable quantum tunneling, neighboring wells should be placed a distance $d \lesssim a$ away from each other.

III.1.2 Exercise

Using the linear approximation provided in Equation 20, we have:

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

Taking GaAs as reference, we have that $E_C(\mathrm{GaAs}) = 0\,(\mathrm{meV})$ and $E_C(\mathrm{AlAs}) = 230\,\mathrm{meV}$. Substituting,

$$E_C(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}) = 189\,\mathrm{meV} = 230x\,\mathrm{meV}(+0)$$

$$x = \frac{189}{230} \approx 0.822$$

Hence, we are aiming for a composition of $\mathrm{Al}_{0.822}\mathrm{Ga}_{0.178}\mathrm{As}$.

III.1.3 Question

1. As shown in section **II.2 The Finite Square Well**, the energy levels are proportional to a^{-2}, so the energy levels will decrease when the well is made wider.

2. As the energy levels decrease the differences between them scale by the same factor, so the spacing between the energy levels decreases as well.

III.2 Two-Well System

III.2.1 Question

1. The probability density of the wavefunctions is no longer symmetrical in a single well because of asymmetric boundary conditions. Let us focus on the portion of the wavefunction in the right well. The new $n = 1$ and $n = 2$ states are unimodal, with a single point of maximum probability near (but not exactly at) the center of the well. The new $n = 3$ and $n = 4$ states are bimodal, with two points of maximum probability at the left and right sides of the well.

2. Based on the modality of the probability densities, it seems that the old $n = 1$ state has split into the new $n = 1$ and $n = 2$ states, since all of these states are unimodal within a single well. It also seems that the old $n = 2$ state has split into the new $n = 3$ and $n = 4$ states, since all of these states are bimodal within a single well.

III.2.2 Exercise

The potential is even. Similar to the assertion made in the problem text in section **II.2 The Finite Square Well**, this tells us WLOG that eigenstates of the well are either even or odd. We shall only focus on the odd case here. This immediately tells us that $q(x) = -f(x)$, $j(x) = -g(x)$, and that $h(x)$ is odd. Let's focus on the region $x > 0$ for our analysis. We demand the wavefunction must be continuous, differentiable, and normalizable for finite energies. This gives us the following boundary conditions:

- $h(0) = 0$
- $g(b/2) = h(b/2)$
- $g'(b/2) = h'(b/2)$
- $f(b/2 + a) = g(b/2 + a)$
- $f'(b/2 + a) = g'(b/2 + a)$
- $\lim_{x\to\infty} f(x) = 0$

In the free regions with $V = 0$, with $\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$:

$$h(x) = A_h e^{\kappa x} + B_h e^{-\kappa x}$$

$$f(x) = A_f e^{\kappa x} + B_f e^{-\kappa x}$$

In the bound region with $V = -V_0$, with $l \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar}$:

$$g(x) = C \sin(lx) + D \cos(lx)$$

Applying our boundary conditions from the list above, we have:

- $A_h + B_h = 0$
- $C \sin(lb/2) + D \cos(lb/2) = A_h e^{\kappa b/2} + B_h e^{-\kappa b/2}$

- $l(C\cos(lb/2) - D\sin(lb/2)) = \kappa\big(A_h e^{\kappa b/2} - B_h e^{-\kappa b/2}\big)$
- $A_f e^{\kappa(b/2+a)} + B_f e^{-\kappa(b/2+a)} = C\sin(l(b/2+a)) + D\cos(l(b/2+a))$
- $\kappa\big(A_f e^{\kappa(b/2+a)} - B_f e^{-\kappa(b/2+a)}\big) = l(C\cos(l(b/2+a)) - D\sin(l(b/2+a)))$
- $A_f = 0$

With six unknowns and six boundary conditions, we can solve for the unknowns. A start to the solution can be summarized as follows:

$$\frac{l}{\kappa}\tanh(\kappa b/2) = \frac{C\sin(lb/2) + D\cos(lb/2)}{C\cos(lb/2) - D\sin(lb/2)}$$

$$\tan(l(b/2+a)) = \frac{\frac{l}{\kappa}D - C}{\frac{l}{\kappa}C + D}$$

These should be solved numerically for C and D. Then, the results can be plugged back in to the boundary conditions to solve for $A_h = -B_h$ as well as B_f. After that, we use the fact that the wavefunction is odd to learn the result for the $x < 0$ region as well. At this point, we will have a non-normalized but quantized family of wavefunctions. Finally, we use the constraint that $\int_{-\infty}^{\infty} |\Psi(x)|^2 \, \mathrm{d}x = 1$ to unambiguously learn the family of solutions to the system.

III.2.3 Question

1. We should make the barriers between the wells thinner, as this increases the probability of a particle tunneling through the potential barrier (recall that the wavefunction exponentially attenuates in forbidden regions). As given in **III.2.2**, the potential of a two well system is a piecewise function

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

   where b is the width of the barrier coupling both walls. We can see that as b becomes larger, the potential $-V_0$ encapsulates a larger "region" meaning that it is more likely that a particle is in that region. As b becomes bigger, it makes it harder for a particle to pass through this region. Contrarily, when b becomes smaller, it is more likely that a particle can pass through that region as the probability density is proportional to $|\psi|^2$.

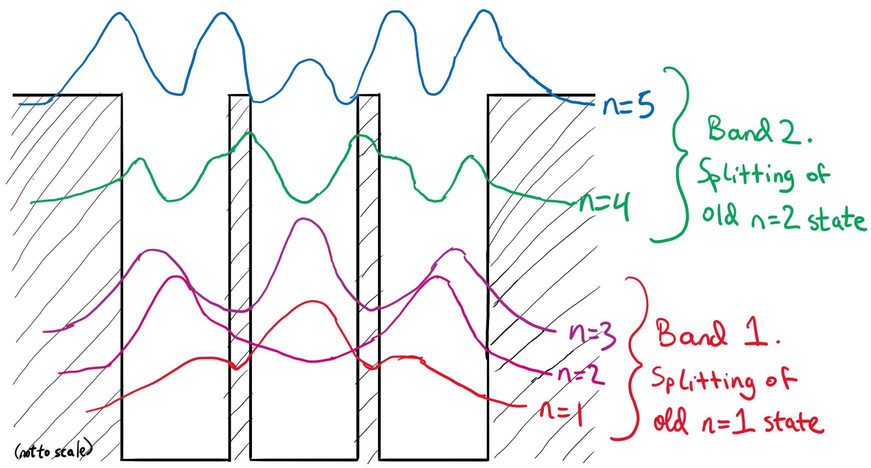
2. Yes, there is a tradeoff. As thickness is increased, the probability of tunneling decreases, but it is easier and less time consuming to make, so one must find the right balance.

III.3 Three-Well System

III.3.1 Question

1. Initially, the waves are that of a single well design of either $n = 1$ or $n = 2$ energy levels. Once these waves pass through the quantum barrier, their energy slowly turns into an exponential function (as shown in above examples) and then moves back to a normal potential well solution when in the next well. The addition of these two wells also splits the $n = 1$ state into a wavefunction with $n = 1, 2, 3$ states while the $n = 2$ state splits into a doublet of $n = 4$ and $n = 5$ states.

2. The old $n = 1$ state has split into the new $n = 1, 2, 3$ triplet. The old $n = 2$ state has split into the new $n = 4, 5$ doublet.



3. No, 3 of the new states correspond to the old $n = 1$ state while only 2 of the new states correspond to the old $n = 2$ state. This is because the splitting of the old $n = 2$ state produces a "$n = 6$" state that exceeds the potential of the system, meaning that state is a scattering state instead of a bound state. The implication is that a particle will be more likely to escape the system if it is excited onto a high enough energy state. In other words, compared to the systems discussed earlier, the particle is less likely to stay within the wells.

III.3.2 Question

The system approaches the behavior of an infinite periodic potential lattice, i.e. a crystal structure. The energy levels keep splitting until they form several energy bands, each band being comprised of many extremely closely spaced energy levels (appears continuous at relevant energies). This kind of behavior is responsible for the electronic band structure of solids.

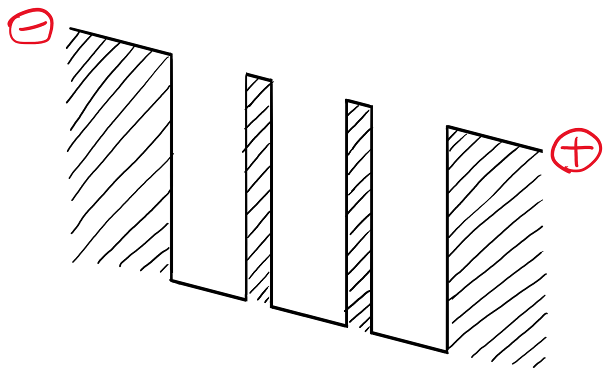
III.4 Biased Three-Well Active Region

III.4.1 Exercise

Note that if $\tan\theta = c$, then $\cos\theta = \sqrt{\frac{1}{1+c^2}}$.

$$V(x) = \begin{cases} cx & |x| > \sqrt{\frac{1}{1+c^2}}\left(\frac{3}{2}a + b\right) \\ cx - V_0 & \sqrt{\frac{1}{1+c^2}}\left(\frac{1}{2}a + b\right) < |x| < \sqrt{\frac{1}{1+c^2}}\left(\frac{3}{2}a + b\right) \\ cx & \sqrt{\frac{1}{1+c^2}}\left(\frac{1}{2}a\right) < |x| < \sqrt{\frac{1}{1+c^2}}\left(\frac{1}{2}a + b\right) \\ cx - V_0 & |x| < \sqrt{\frac{1}{1+c^2}}\left(\frac{1}{2}a\right) \end{cases}$$

III.4.2 Question

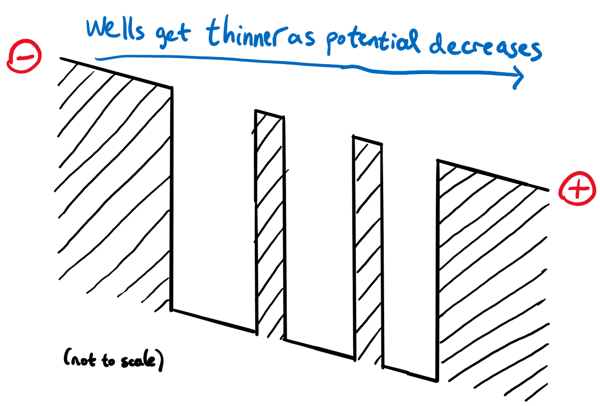


Recall that the graph shows potential energy (not to be confused with electric potential). Since for electrons $E \sim -eV$ (where $e > 0$), the higher energy side should have the negative voltage. Hence, the lower end is (+), and the higher end is (-).

III.4.3 Question

1. Unlike the wells in figure 3, the biased wells are at different potentials compared to each other. Hence, if we look at each well separately (ignoring coupling effects), the energy levels will not line up across all the wells, but will rather tend to be set distances from the bottoms of each well.

2. In the infinite well system, $E \propto a^{-2}$, where a is well thickness. In order to make energy levels line up better across the device, we should decrease the thickness of the lower potential wells. This will make the energy levels tend to be higher, which is qualitatively motivated by the energy levels of the infinite square well. In summary, the higher potential wells should be thicker, and the lower potential wells should be thinner.



III.4.4 Question

1. It will be above the tops of the middle and right-most wells, since the red line is higher than the tops of those wells if it is extended horizontally. Thus, if tunneling occurs, then the electron will no longer be in a bound state, but rather a scattering state. This means that there is a significant probability that the electron leaves the device (as we can see from the time evolution of the wavefunction).

2. When the well is highly biased, the wells and barriers will get thinner, with the thickness proportional to $\sqrt{\frac{1}{1+c^2}}$. The decrease in well width increases the energy of the eigenstates, and the decrease in barrier width means the wavefunction attenuates less in tunneling. Hence, higher bias makes tunneling easier. With higher bias, the electron transport rightwards through the device will occur at a faster rate.

3. There is an important trade-off to consider. Higher bias results in better electron transport but also a higher probability that the electron scatters away. Lower bias results in a higher probability that the electron remains bound (and is retained in the device), but at the cost of slower electron transport.

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

III.5.1 Question

1. The electron begins its journey through the device at the far left of the diagram, when it is introduced to the first injector region. It tunnels through the injector region until it reaches the active region, when the electron emits a photon in the (slow) $n = 3 \to 2$ transition. After it emits a photon here, its energy decreases, and its wavefunction changes to one of a lower energy state. Then, it emits a phonon in the (fast) $n = 2 \to 1$ transition. Once in the $n = 1$ state, it tunnels through the next injector region, and the process repeats.

   Note that the active region models a simple 3-state laser. Since the $n = 3 \to 2$ transition is slow but the $n = 2 \to 1$ transition is fast, there will be a population inversion, where the $n = 3$ state has a higher population than the $n = 2$ state. With the population inversion created, lasing can happen the same way as in a normal laser, by stimulated emission in the $n = 3 \to 2$ transition.

2. The multiple wells in the injector region ensures good electron transport through the system, given that the energy levels line up between adjacent wells. Because we want energy levels to line up as well as possible, there is much less flexibility in setting the widths of the wells in the injector region compared to in the active regions.

3. A single electron will cascade down the system, resulting in an emission in each active region. Since there are multiple active regions throughout the device, the single electron cascading down the system will result in multiple emissions of light. The usefulness of the quantum cascade laser essentially allows a high energy electron to radiate in multiple stages, with an easily controllable frequency based on the concentration of AlGaAs.

III.5.2 Question

Parameters:

- x, the concentration of AlGaAs in $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$. This controls V_0, the depth of the well. It's given in section **III.1.2 Exercise** that we want $V_0 = 189\,\mathrm{meV}$, which led to a result of $x = 0.822$, in order to "minimize lattice strain while sufficiently containing the $n = 1$ and $n = 2$ eigenstates."

- a, the width of the wells. This is variable for the different wells in the biased system, since it should be thinner for lower potential wells and thicker for higher potential wells. There's a trade-off between tunneling and minimum well thickness, where thinner wells allow for easier tunneling but are harder to grow. See section **III.2.3 Question**.

- b, the width of the barriers. Note that both a and b should be at least three atomic layers thick ($\sim 3 - 9$Å).

- c, the slope of the potential in the biased system. There's a trade-off here as well. A higher biased well will reduce the thickness of the potential barriers, which allows for easier tunneling and electron transport through the device. However, it also means that electrons are more likely to enter a scattering state and escape the device.

We can tune a to adjust the emitted wavelength of the laser. Also, we should design the $n = 2 \to 1$ transition in the active region such that it results in minimal energy loss in the system through phonon emission.