# P3317 HW from Lecture 10+11 and Recitation 6

**Due Thursday October 11 – Note the delay due to Fall Break**

**Solution 0.0.**

| Terms | Count |
|---|---|
| (Too) Long | 5 |
| Tedius | 3 |
| Frustrating | 2 |
| Hard | 2 |
| Cool | 1 |
| Horrible | 1 |
| Obnoxious | 1 |
| Difficult | 1 |
| Fun | 1 |
| Interesting | 1 |
| Fair | 1 |
| Confusing | 1 |
| Good | 1 |
| Necessary | 1 |
| Useful | 1 |

| Hours | Count |
|---|---|
| 4 | 1 |
| 4.5 | 1 |
| 5 | 1 |
| 5 | 3 |
| 6 | 1 |
| 7 | 1 |
| 8 | 1 |
| 10 | 2 |
| 12 | 1 |

**Problem 1. Quantum Cryptography**

[This was adapted from a 2014 P3317 final exam problem. It is a little lengthy – but is really cool.]

Cryptography involves sending a message to a correspondent while minimizing the risk of interception by an unwanted outsider. Measuring a quantum system disturbs it – a feature which can be used as part of a cryptography scheme.

Following convention we will label the person sending the message as "Alice," and use the symbol $A$ to label quantities associated with her. The receiver is "Bob." A spy trying to listen in on the conversation is "Cathy." The message consists of a sequence of $+1$ and $-1$'s. For example, letting $+$ denote a $+1$ and $-$ denote a $-1$, a message could be $++---++$.

Consider a spin 1/2 particle. The spin operator is $\mathbf{S} = (\hbar/2)\vec{\sigma}$, where the set $\sigma_i, i = x, y, z$ are Pauli matrices. We write $|\sigma_z = +1\rangle$ and $|\sigma_z = -1\rangle$ for the eigenstates of $S_z$ with eigenvalues $\hbar/2$ and $-\hbar/2$.

Consider a particle in the state $|\sigma_z = +1\rangle$. As in our analysis of Bells inequalities, one can measure the component of the spin along an axis $u$ in the $(x, z)$ plane, defined by the unit vector

$$\hat{\mathbf{u}} = \cos(\theta)\hat{\mathbf{z}} + \sin(\theta)\hat{\mathbf{x}}. \tag{1}$$

The corresponding operator is

$$S_u = \mathbf{S} \cdot \hat{\mathbf{u}} = \frac{\hbar}{2} \left( \cos(\theta) \sigma_z + \sin(\theta) \sigma_x \right). \tag{2}$$

The possible results of the measurement are $+\hbar/2$ and $-\hbar/2$.

One sees this by noting that the relevant operator is

$$S_u = \frac{\hbar}{2} \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ \sin(\theta) & -\cos(\theta) \end{pmatrix}. \tag{3}$$

We let $\lambda_1$ and $\lambda_2$ be the eigenvalues. The trace of this matrix is $\lambda_1 + \lambda_2 = 0$ and the determinant is $\lambda_1 \lambda_2 = -\hbar^2/4$. Thus the eigenalues are $\lambda_2 = -\lambda_1 = \hbar/2$.

**1.1.** The eigenstates of the observable in Eq. (2) can be written

$$\begin{aligned} |\sigma_u = +1\rangle &= \cos(\phi)|\sigma_z = +1\rangle + \sin(\phi)|\sigma_z = -1\rangle && (4) \\ |\sigma_u = -1\rangle &= -\sin(\phi)|\sigma_z = +1\rangle + \cos(\phi)|\sigma_z = -1\rangle. && (5) \end{aligned}$$

Express $\phi$ in terms of $\theta$.

**Solution 1.1.** (2 points)
To find the relationship between $\theta$ and $\phi$, we must solve

$$\begin{pmatrix} \cos(\theta) - 1 & \sin(\theta) \\ \sin(\theta) & -\cos(\theta) - 1 \end{pmatrix} \begin{pmatrix} \cos(\phi) \\ \sin(\phi) \end{pmatrix} = \begin{pmatrix} \cos(\phi) \\ \sin(\phi) \end{pmatrix}. \tag{6}$$

While there are many ways to do this, one elegant approach is to multiply the first equation by $\cos(\phi)$ and the second by $\sin(\phi)$ and add them to find

$$\begin{aligned} 0 &= \cos(\phi) \left[ (\cos(\theta) - 1) \cos(\phi) + \sin(\theta) \sin(\phi) \right] && (7) \\ &\quad + \sin(\phi) \left[ \sin(\theta) \cos(\phi) - (\cos(\theta) + 1) \sin(\phi) \right] \\ &= \cos(\theta)[\cos^2(\phi) - \sin^2(\phi)] + \sin(\theta)[2\cos(\phi)\sin(\phi)] - [\cos^2(\phi) + \sin^2(\phi)]. && (8) \end{aligned}$$

We then use our half angle identities to rewrite this as

$$0 = \cos(\theta)\cos(2\phi) + \sin(\theta)\sin(2\phi) - 1. \tag{9}$$

A second round of trigonometric identities gives

$$0 = \cos(\theta - 2\phi) - 1, \tag{10}$$

or $\phi = \theta/2$.
An alternative approach is to look up this result in homework 4.

**1.2.** In terms of $\phi$, what is the probability $p_+$ that the measurement yields $+\hbar/2$?

**Solution 1.2.** (1 point) According to the axioms of measurement, this probability is the square of the overlap between the initial state and the state which is the eigenvector of the operator,

$$p_+ = \cos^2(\phi). \tag{11}$$

**1.3.** If the measurement yields $+\hbar/2$, what will the spin state be immediately after the measurement?

**Solution 1.3.** (1 point) According to the axioms of measurement the spin will be in the state $|\sigma_u = +1\rangle$.

**1.4.** In terms of $\phi$, what is the probability $p_-$ that the measurement yields $-\hbar/2$?

**Solution 1.4.** (1 point) According to the axioms of measurement

$$p_- = \sin^2(\phi). \tag{12}$$

**1.5.** If the measurement yields $-\hbar/2$, what will the spin state be immediately after the measurement?

**Solution 1.5.** (1 point) According to the axioms of measurement the spin will be in the state $|\sigma_u = -1\rangle$.

**1.6.** Suppose after measuring the observable in Eq. (2) and finding $+\hbar/2$ one measures $S_z$. What is the probability $q_+$ that one finds $\hbar/2$ for this second measurement?

**Solution 1.6.** (1 point) According to the axioms of measurement, this probability is the square of the overlap between the initial state and the state which is the eigenvector of the operator,

$$q_+ = \cos^2(\phi). \tag{13}$$

**1.7.** Suppose after measuring the observable in Eq. (2) and finding $+\hbar/2$ one measures $S_z$. What is the probability $q_-$ that one finds $-\hbar/2$ for this second measurement?

**Solution 1.7.** (1 point) According to the axioms of measurement, this probability is the square of the overlap between the initial state and the state which is the eigenvector of the operator,

$$q_- = \sin^2(\phi). \tag{14}$$

**1.8.** Imagine a sequence where one begins with the spin in the $|\sigma_z = +1\rangle$, measures $S_u$, then measures $S_z$. Show that the total probability of finding $+\hbar/2$ for this second measurement is

$$P_{++}(\theta) = p_+q_+ + p_-q_- = \frac{1+\cos^2(\theta)}{2}. \tag{15}$$

**Solution 1.8.** (1 point)

$$
\begin{aligned}
P_{++}(\theta) &= p_+q_+ + p_-q_- &(16)\\
&= \cos^4(\phi) + \sin^4(\phi) &(17)\\
&= \frac{[\cos^2(\phi)+\sin^2(\phi)]^2}{2} + \frac{[\cos^2(\phi)-\sin^2(\phi)]^2}{2} &(18)\\
&= \frac{1-\cos^2(2\phi)}{2} &(19)\\
&= \frac{1-\cos^2(\theta)}{2}. &(20)
\end{aligned}
$$

**1.9.** Assuming now that the initial state is $|\sigma_z = -1\rangle$. One measures $S_u$, then measures $S_z$. What is the total probability, $P_{--}(\theta)$ of finding $-\hbar/2$ for this second measurement?

**Solution 1.9.** (1 point) By symmetry,

$$P_{--} = P_{++} \tag{21}$$

**1.10.** Imagine now that we have two spins in the state

$$|\Sigma\rangle = \frac{1}{\sqrt{2}}\Big[|\sigma_z^a = +1\rangle \otimes |\sigma_z^b = +1\rangle + |\sigma_z^a = -1\rangle \otimes |\sigma_z^b = -1\rangle\Big]. \tag{22}$$

We saw this state when discussing Bell's inequalities. Show that this can also be written as

$$|\Sigma\rangle = \frac{1}{\sqrt{2}}\Big[|\sigma_x^a = +1\rangle \otimes |\sigma_x^b = +1\rangle + |\sigma_x^a = -1\rangle \otimes |\sigma_x^b = -1\rangle\Big]. \tag{23}$$

**Solution 1.10.** (1 point) I will do one better, and show that for any direction $\hat{\mathbf{u}}$,

$$|\Sigma\rangle = \frac{1}{\sqrt{2}}\Big[|\sigma_u^a = +1\rangle \otimes |\sigma_u^b = +1\rangle + |\sigma_u^a = -1\rangle \otimes |\sigma_u^b = -1\rangle\Big]. \tag{24}$$

To show this I begin with Eq. (24) and simply substitute our expression for $|\sigma_u = \pm 1\rangle$,

$$
\begin{aligned}
|\Sigma\rangle &= \frac{1}{\sqrt{2}}\Big[(\cos(\phi)|\sigma_z^a = +1\rangle + \sin(\phi)|\sigma_z^a = -1\rangle) \otimes \Big(\cos(\phi)|\sigma_z^b = +1\rangle + \sin(\phi)|\sigma_z^b = -1\rangle\Big)\\
&\quad + (-\sin(\phi)|\sigma_z^a = +1\rangle + \cos(\phi)|\sigma_z^a = -1\rangle) \otimes \Big(-\sin(\phi)|\sigma_z^b = +1\rangle + \cos(\phi)|\sigma_z^b = -1\rangle\Big)\Big] &(25)\\
&= \frac{1}{\sqrt{2}}\Big[(\cos^2(\phi) + \sin^2(\phi))|\sigma_z^a = +1\rangle \otimes |\sigma_z^b = +1\rangle\\
&\quad + (\cos(\phi)\sin(\phi) - \sin(\phi)\cos(\phi)|\sigma_z^a = -1\rangle \otimes |\sigma_z^b = +1\rangle\\
&\quad + (\cos(\phi)\sin(\phi) - \sin(\phi)\cos(\phi)|\sigma_z^a = -1\rangle \otimes |\sigma_z^b = -1\rangle\\
&\quad + (\sin^2(\phi) + \cos^2(\phi)|\sigma_z^a = -1\rangle \otimes |\sigma_z^b = -1\rangle] &(26)\\
&= \frac{1}{\sqrt{2}}\Big[|\sigma_z^a = +1\rangle \otimes |\sigma_z^b = +1\rangle + |\sigma_z^a = -1\rangle \otimes |\sigma_z^b = -1\rangle\Big]. &(27)
\end{aligned}
$$

Taking $\phi = \pi/4$ yields the desired result.
Of course, I expect most students will just do the case asked.

**1.11.** The pair of particles $(a, b)$ is prepared in the spin state $|\Sigma\rangle$ in Eq. (22). As the two particles move away from one another, this spin state remains unchanged unless a measurement is made. Alice measures the spin component of $a$ along an axis $u_a$ defined by the angle $\theta_a$. What are the possible results and the corresponding probabilities in the two cases $\theta_a = 0$ and $\theta_a = \pi/2$. These respectively correspond to the $\hat{z}$ and $\hat{x}$ axis.

**Solution 1.11.** (1 point) Alice will find either $+\hbar/2$ or $-\hbar/2$, each with probability 1/2 – regardless of which axis she measures along.

**1.12.** After Alice's measurement, the spin state of the two particles will depend on the result of the measurement. For example, if Alice measures along $\hat{z}$ and finds $\hbar/2$ the spins will be in the state

$$|\uparrow\uparrow\rangle = |\sigma_z^a = +1\rangle \otimes |\sigma_z^b = +1\rangle.$$

If Alice measures along $\hat{z}$ and finds $-\hbar/2$ what will the spin state be?

**Solution 1.12.** (1 point) The spins will be in the state

$$|\downarrow\downarrow\rangle = |\sigma_z^a = -1\rangle \otimes |\sigma_z^b = -1\rangle$$

**1.13.** If Alice measures along $\hat{x}$ and finds $\hbar/2$ the spins will be in the state

$$|\rightarrow\rightarrow\rangle = |\sigma_x^a = +1\rangle \otimes |\sigma_x^b = +1\rangle$$

. If Alice measures along $\hat{x}$ and finds $-\hbar/2$, what will the spin state be?

**Solution 1.13.** (1 point) The spins will be in the state

$$|\leftarrow\leftarrow\rangle = |\sigma_x^a = -1\rangle \otimes |\sigma_x^b = -1\rangle$$

**1.14.** After Alice's measurement, Bob measures the spin of particle $b$ along an axis $u_b$ defined by the angle $\theta_b$. Give the possible results of Bob's measurement and their probabilities in terms of Alice's results in the following four configurations:

1. $\theta_a = 0, \theta_b = 0$
2. $\theta_a = 0, \theta_b = \pi/2$
3. $\theta_a = \pi/2, \theta_b = 0$
4. $\theta_a = \pi/2, \theta_b = \pi/2$

**Solution 1.14.** (4 points – 1/2 for each of the eight cases) These results are best summarized in a table

| Alice's axis $\theta_a$ | Bob's axis $\theta_b$ | Alice's Result | Bob's Result | Bob's Probability |
|---|---|---|---|---|
| 0 | 0 | $+\hbar/2$ | $+\hbar/2$ | 1 |
| 0 | 0 | $+\hbar/2$ | $-\hbar/2$ | 0 |
| 0 | $\pi/2$ | $+\hbar/2$ | $+\hbar/2$ | 1/2 |
| 0 | $\pi/2$ | $+\hbar/2$ | $-\hbar/2$ | 1/2 |
| $\pi/2$ | 0 | $+\hbar/2$ | $+\hbar/2$ | 1/2 |
| $\pi/2$ | 0 | $+\hbar/2$ | $-\hbar/2$ | 1/2 |
| $\pi/2$ | $\pi/2$ | $+\hbar/2$ | $+\hbar/2$ | 0 |
| $\pi/2$ | $\pi/2$ | $+\hbar/2$ | $-\hbar/2$ | 1 |

(28)

**1.15.** In which of the four cases are the measurements on $a$ and $b$ guaranteed to give the same result?

**Solution 1.15.** (1 point) Whenever Bob and Alice choose the same axis they find the same result.

**1.16.** A spy, Cathy, sits between the source and Bob. She measures the spin of particle $b$ along an axis $u_c$ defined by angle $\theta_c$, then lets the spin continue on to Bob. Suppose $\theta_a = 0$. In terms of $\theta_c$, and Alice's findings, what are the possible results of Cathy's measurements, and what are their possibilities? [You may find it useful to take advantage of your results from earlier questions.]

**Solution 1.16.** (2 points: 1/2 for each of the four cases) Using our previous results, if Alice measures $+\hbar/2$ then Cathy will measure $+\hbar/2$ with probability $p_+ = \cos^2(\theta_c/2)$, and $-\hbar/2$ with probability $p_- = \sin^2(\theta/2)$. Conversely if Alice measures $-\hbar/2$ then Cathy will measure $-\hbar/2$ with probability $p_+ = \cos^2(\theta_c/2)$, and $+\hbar/2$ with probability $p_- = \sin^2(\theta/2)$.

**1.17.** After Cathy's measurement, Bob measures the spin of $b$ along the axis $\theta_b = 0$. In terms of Cathy's results, what does Bob find, and with what probability? [You may find it useful to take advantage of your earlier results.]

**Solution 1.17.** (2 points: 1/2 for each of the four cases) Using our previous results, if Cathy measures $+\hbar/2$ then Bob will measure $+\hbar/2$ with probability $q_+ = \cos^2(\theta_c/2)$, and $-\hbar/2$ with probability $q_- = \sin^2(\theta/2)$. Conversely if Cathy measures $-\hbar/2$ then Bob will measure $-\hbar/2$ with probability $q_+ = \cos^2(\theta_c/2)$, and $+\hbar/2$ with probability $q_- = \sin^2(\theta/2)$.

**1.18.** Suppose that $\theta_a = \theta_b = 0$. As before, Cathy measures the spin along the direction $\theta_c$. What is the probability $P(\theta_c)$ that Alice and Bob find the same result after Cathy's measurement?

**Solution 1.18.** (1 point) This is just our old friend

$$P(\theta_c) = P_{++} = P_{--} = \frac{1 + \cos^2(\theta_c)}{2} \tag{29}$$

**1.19.** What is the expectation value of $P(\theta_c)$ if Cathy chooses $\theta_c$ at random in the interval $[0, 2\pi]$ with uniform probability?

**Solution 1.19.** (1 point) The average of $\cos^2(\theta_c)$ is 1/2, so

$$\langle P \rangle = \frac{1}{2\pi} \int_0^{2\pi} P(\theta_c) = 3/4. \tag{30}$$

**1.20.** What is the expectation value of $P(\theta_c)$ if Cathy chooses $\theta_c$ to be either 0 or $\pi/2$, each with probability 1/2.

**Solution 1.20.** (1 point) Conveniently this

$$\langle P \rangle = \frac{P(0) + P(\pi/2)}{2} = 3/4. \tag{31}$$

We can now explain the quantum cryptography procedure

1. Alice prepares her $n$ bit message
2. Alice, who controls the source, prepares an ordered sequence of $N \gg n$ pairs in the spin state $|\Sigma\rangle$. She sends all the $b$ spins to Bob and keeps the $a$ spins.
3. For each spin they collect, Alice and Bob measure either the $x$ or the $z$ component. For each spin they independently choose the $x$ or $z$ direction at random with probability $p = 1/2$. Alice's choice and Bob's choice are independent. The both register all their results.
4. Bob selects a subset of his measurements (say $N/2$ of them). He calls Alice on the telephone, and gives this list to Alice. He includes the axis, and the result of the measurement
5. Alice compares, for these $N/2$ spins, her axes and her results. By doing so she can tell if a spy is present. If a spy is spotted they abort the transmission.
6. For the other $N/2$ spins, Bob tells Alice which axes he measured, but he does not tell her his results.
7. Alice calls Bob on the phone, and ...

**1.21.** How can Alice be sure that a spy is present?

**Solution 1.21.** (1 point) She looks at qbits where both Alice and Bob chose the same axis. If they did not measure the same state, there must have been an easedropper.

**1.22.** What is the probability that an operating spy will escape being detected? Calculate this probability for $N/2 = 200$. Make some reasonable assumptions. For example, assume Cathy randomly chooses $\theta_c$ independently for each spin, and use the results of 1.19 or 1.20. Explicitly state all your assumptions.

**Solution 1.22.** (2 points) The best argument is that for a given spin, Cathy has a probability of 1/8 of being caught: half the time Alice and Bob get the same result, and she gets caught on only 3/4 of those. Thus the probability that she is lucky all 200 times is $(7/8)^{200} = 2.5 \times 10^{-12}$. An acceptable argument is that of the 200 results that Bob shares with Alice, roughly 100 of them will have the same axis. For each of these, Cathy has a 75% chance of not being detected. Thus the probability that she is lucky all 100 times is $(3/4)^{100} = 3 \times 10^{-13}$.
Regardless, for $N/2 = 200$ she will get caught.

**1.23.** After one attempt to communicate, Alice measured $1 : x+, 2 : z+, 3 : z-, 4 : z+, 5 : x+, 6 : x-, 7 : z+, 8 : x+, 9 : x-, 10 : z-, 11 : x+, 12 : z+$ the number represents which spin, the letter represents the axis, and the $\pm$ gives the result of the measurement. Bob reported to Alice half of his results $2 : x+, 5 : x+, 8 : x-, 9 : z+, 11 : z+, 12 : z-$. Alice declared that there was a spy. How did she know?

**Solution 1.23.** (1 point) Alice noticed that on spin 8 and 12 she had the same axes as Bob, but they found different results. This was the smoking gun for a spy.

**1.24.** In as separate attempt to communicate, Alice measured $1 : x+, 2 : x-, 3 : z+, 4 : x+, 5 : z-, 6 : z-, 7 : x+, 8 : z+, 9 : z+, 10 : z-, 11 : x+, 12 : x-$. Bob reports $1 : x+, 3 : x-, 4 : z-, 7 : x+, 10 : x+, 11 : x+$. Alice decides that it was unlikely that a spy was listening in. What is the probability that a spy was listening?

**Solution 1.24.** (1 point) There were 3 opportunities for a spy to have messed up. The probability that a spy listening in would not have been caught was $p = (3/4)^3$ =42%. By our ordinary (and imprecise) reasoning about probabilities, we would typically argue that the probability $p$ also represents the probability that there was not a spy. So for this short sequence she will not be all that certain.

**Solution 1.24 (Further Details).** While that answer is all I was looking for, one can use Bayes' theorem to make a more sophisticated argument. Bayes' theorem starts with the obvious statement that the probability of both $A$ and $B$ is that the conditional probability of $A$ given $B$ times the probability of $B$

$$P(A \cup B) = P(A|B)P(B). \tag{32}$$

The same argument gives

$$P(A \cup B) = P(B|A)P(A). \tag{33}$$

Thus we know

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}. \tag{34}$$

Let $A$ denote the presence of a spy, and $P(A)$ is the probability that a spy listens in on any given conversation. Let $B$ represent the particular outcome that Alice and Bob found. We want to know $P(A|B)$, the probability that the spy was listening, given the observed outcome.
If there was a spy, we would be less likely to find this particular pattern than if there were no spy. If we let $P(B|\bar{A})$ be the probability of $B$ in the absence of a spy, then

$$\frac{P(B|A)}{P(B|\bar{A})} = p = (3/4)^3 . \tag{35}$$

Next we note

$$P(B) = P(B|A)P(A) + P(B|\bar{A})\bar{A} = P(B|A)(P(A) + [1 - P(A)]/p), \tag{36}$$

and hence

$$P(A|B) = \frac{pP(A)}{1 + (p-1)P(A)}. \tag{37}$$

At this point we need one more piece of modeling – known as a "prior." We need an estimate of how often spies are listening in on our conversations. If we are paranoid, we would say $P(A) = 1$ – in which case we would conclude that there was a spy, and they were just lucky. If we are overconfident, we would say $P(A) = 0$, and there certainly is not a spy, and our experiment just confirmed this. If we were an empiricist, we would carry out multiple experiments, and estimate $P(A)$ from how often we catch spies. I will take the middle road, and assume that half the time a spy is listening in, this would give

$$P(A|B) = \frac{p}{1+p}, \tag{38}$$

which for small $p$ this gives our previous result $P(A|B) \approx p$.

**1.25.** In this second case [where Alice measured $1 : x+, 2 : x-, 3 : z+, 4 : x+, 5 : z-, 6 : z-, 7 : x+, 8 : z+, 9 : z+, 10 : z-, 11 : x+, 12 : x-$ and Bob reported $1 : x+, 3 : x-, 4 : z-, 7 : x+, 10 : x+, 11 : x+$], Bob reports the following axes: $2 : x, 5 : x, 6 : x, 8 : z, 9 : x, 12 : x$. Alice wants to send the message $(+, -)$. What can she tell Bob on the phone to securely transmit this message? What will Bob do?

**Solution 1.25.** (2 points) There are more than one protocols which work, but one simple one is that Alice tells Bob to look at spin #8 and spin #12, in that order. She tells him that those spins will contains the bits that she wants to send. Since they measured the same axes on those bits, Alice knows that when Bob looks at spin #8 he will see a +, and when he looks at #12 he will see a -.

**Problem 2.** We wish to use the variational principle to estimate the ground state energy of the Hydrogen atom.

**2.1.** Using the techniques we have previously studied, adimensionalize the time independent Schrodinger equation for the electron in a Hydrogen atom

$$E\psi(r) = -\frac{\hbar^2}{2m}\nabla^2\psi(r) - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}\psi(r). \tag{39}$$

Call your scaled coordinate $s$.

**Solution 2.1** (4 points)**.** We wish to make the replacement:

$$E = \mathcal{E}E_0, \qquad r = yr_0, \tag{40}$$

giving:

$$E_0\mathcal{E}\psi(s) = -\frac{\hbar^2}{2mr_0^2}\partial_s^2\psi(s) - \frac{e^2}{4\pi\epsilon_0 r_0}\frac{1}{s}\psi(s). \tag{41}$$

We adimensionalize this by solving the two equations

$$\begin{aligned} E_0 &= \alpha\frac{\hbar^2}{2mr_0^2} \\ \frac{\hbar^2}{2mr_0^2} &= \beta\frac{e^2}{4\pi\epsilon_0 r_0}, \end{aligned} \tag{42}$$

where $\alpha$ and $\beta$ are completely arbitrary numbers. Common choices are likely to be $\alpha = 1, 2$ and $\beta = 1, 4\pi, 2\pi$.

I will quote results for $\alpha = \beta = 1$, which yields

$$\mathcal{E}\psi(s) = -\partial_s^2\psi(s) - \frac{1}{s}\psi(s). \tag{43}$$

Eq. (42) is solved by:

$$r_0 = \frac{2\pi\epsilon_0\hbar^2}{e^2 m}, \qquad E_0 = \frac{2e^4 m}{(4\pi\epsilon_0)^2\hbar^2}. \tag{44}$$

If you used a different value of $\alpha$ and $\beta$, $r_0$ and $E_0$ will be multiplied by some numbers, but the symbols will all be the same.

**2.2.** Given an arbitrary normalized function of the scaled coordinate, $\psi(s)$, we can use the variational principle to produce an upper bound to the ground state energy of Hydrogen. By normalized, I mean

$$\int d^3s\,|\psi(s)|^2 = 1. \tag{45}$$

Write an expression for this variational bound. The expression will have the form

$$\frac{E}{E_0} = A \int d^3s\, |\nabla\psi(s)|^2 + B \int d^3s\, \frac{|\psi(s)|^2}{s}, \tag{46}$$

where $E_0$ is the energy scale used in adimensionalizing the Schrodinger equation, $A, B$ are dimensionless constants. Find $A$ and $B$.

**Solution 2.2** (3 points)**.** There are a number of approaches. The most elementary involves multiplying Eq. (43) by $\psi(s)^*$ to find:

$$\mathcal{E}|\psi(s)|^2 = -\left(\partial_s^2\psi(s)\right)\psi(s)^* - \frac{1}{s}|\psi(s)|^2, \tag{47}$$

which we can integrate on both sides over all space, and integrate the first term on the RHS by parts (assuming the boundary terms go to zero):

$$\mathcal{E}\int d^3s|\psi(s)|^2 = -\int d^3s\left(\partial_s^2\psi(s)\right)\psi(s)^* - \int d^3s\frac{|\psi(s)|^2}{s}, \tag{48}$$

$$\mathcal{E} = \int d^3s|\partial_s\psi(s)|^2 - \int d^3s\frac{1}{s}|\psi(s)|^2. \tag{49}$$

For my choice of $\alpha$ and $\beta$, I find that $A = 1$ and $B = -1$. Other choices will give different numbers – but they will always just be dimensionless numbers.

**2.3.** We will try the following variational wavefunction

$$\psi(s) = \frac{1}{\sqrt{8\pi\lambda^3}}e^{-s/(2\lambda)}, \tag{50}$$

where $\lambda$ is an undetermined variational parameter. This is is properly normalized as

$$\int d^3s\, |\psi(s)|^2 = 4\pi\int ds\, s^2|\psi(s)|^2 = 1. \tag{51}$$

Calculate the variational energy $E(\lambda)$ in Eq. (46). Just use the symbols, $A$, $B$, and $E_0$. Do not substitute your expressions for these parameters.

**Solution 2.3** (2 points)**.** Performing the integral gives:

$$\frac{E}{E_0} = A\left(\frac{-1}{2\lambda}\right)^2\int d^3s\, |\psi(s)|^2 + B\frac{1}{8\pi\lambda^3}\int d^3s\, \frac{e^{-s/\lambda}}{s}, \tag{52}$$

$$\frac{E}{E_0} = A\frac{1}{4\lambda^2} + B\frac{1}{2\lambda^3}\int ds\, se^{-s/\lambda}, \tag{53}$$

$$\frac{E}{E_0} = A\frac{1}{4\lambda^2} + B\frac{1}{2\lambda^3}\left((-\lambda)[se^{-s/\lambda}]_0^\infty - \int_0^\infty ds\, (-\lambda)e^{-s/\lambda}\right), \tag{54}$$

$$\frac{E}{E_0} = A\frac{1}{4\lambda^2} + B\frac{1}{2\lambda}. \tag{55}$$

Therefore:

$$E(\lambda) = E_0\left(A\frac{1}{4\lambda^2} + B\frac{1}{2\lambda}\right). \tag{56}$$

**2.4.** Minimize $E(\lambda)$ with respect to $\lambda$. Again, just use the symbols $A$, $B$, and $E_0$.

**Solution 2.4** (2 points)**.** To find the minimum energy, we wish to solve $\partial_\lambda E(\lambda) = 0$, ensuring also that it is a minimum:

$$\partial_\lambda E(\lambda)|_{\lambda_0} = 0 = E_0 \left( -A \frac{1}{2\lambda_0^3} - B \frac{1}{2\lambda_0^2} \right), \tag{57}$$

$$\implies \lambda_0 = -\frac{A}{B} \quad (\text{or } \lambda \to \infty). \tag{58}$$

To check that the first solution is indeed a minimum, note that the function goes to +ive infinity at $\lambda = 0$, is negative at $\lambda_0$, and goes to 0 as $\lambda \to \infty$.
The value of the energy at the minimum is

$$E(\lambda_0) = -\frac{E_0}{4} \frac{B^2}{A}. \tag{59}$$

**2.5.** Substitute in your values for $A$, $B$, and $E_0$. What is your bound on the energy in $eV$.

**Solution 2.5** (2 points)**.** This simply involves plugging in your expressions. The result is independent of $\alpha$ and $\beta$, but the intermediate steps do depend on them. One way to organize things is to write

$$E_0 = 2 \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{m}{\hbar} = 2 \left( \frac{1}{137} \right)^2 \left( 0.51 \times 10^6 \text{ eV} \right) \tag{60}$$

$$= 54.3 \text{ eV}, \tag{61}$$

where I have used that the fine structure constant $\alpha = e^2/4\pi\epsilon_0 \hbar c \simeq 137^{-1}$. Plugging this in gives:

$$E_{\text{bound}} = 13.6 \text{ eV}, \tag{62}$$

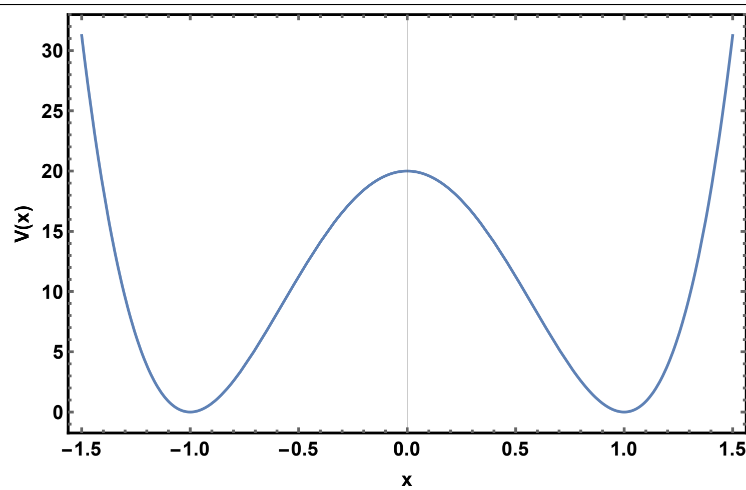
which happens to be right on, due to a fortuitous choice of variational function.

**Problem 3.** Consider the adimensionalized time independent Schrodinger equation for a particle in a double well potential

$$E\psi(x) = -\frac{1}{2}\partial_x^2 \psi(x) + V_0(x^2 - 1)^2 \psi(x). \tag{63}$$

Take $V_0 = 20$.

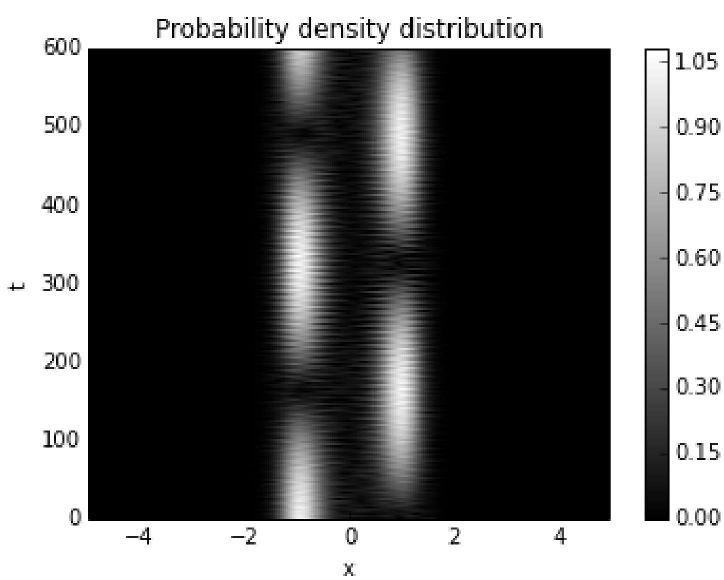
**3.1.** Plot the potential. Label your graph.




**Solution 3.1** (3 points).

**3.2.** Choose a reasonable spatial and temporal discretization (I took $dx = 0.05$ with $x$ running from $-5$ to 5 and $dt = 0.01$, and it seemed to work for me). Make a stationary wave packet of width 0.3, centered at $x = -1$. Numerically integrate the time dependent Schrodinger equation until time $t = 600$. Make a properly labeled density plot where the horizontal axis is position, the vertical axis is time, and the brightness corresponds to $|\psi|^2$.

**Solution 3.2** (5 points: 1 point for having a density plot, 1 point for labeling axes, 3 points for having correct density (partial marks possible), density key is not necessary).




**3.3.** Describe in words what you observe. Is this result consistent with the modeling of Ammonia we used in terms of two-level systems?

**Solution 3.3** (2 points). The particle tunnels back and forth between the two minima. It is always measured to be in one minimum or the other, never somewhere in the middle. This result is consistent with modelling Ammonia as a two-level system. You might also be able to see some small fast oscillations within each well, which correspond to mixing in some higher energy states. Different choices of wave-packets will accentuate or reduce those features, which are not captured by our two-state approximation.

**Problem 4. Feedback**

**4.1.** How long did this homework take?

**4.2.** Which of the following words come to mind when you think about this homework (feel free to add your own words if you have something better): frustrating, fun, tedious, insightful, hard, easy, useful, useless, fair, unfair