PHYS 357 Final Exam. You have 3 hours. You may use 3 pages of notes and a calculator. There are 100 total points available, plus up to 5 bonus points that can be used to make of for points missed elsewhere (so your total score is capped at 100 points). There are 4 problems and a total of 4 pages, not counting the cover sheet.

1. (15 points) Consider a wave function $\Psi(x)$ that is an energy eigenstate for some potential $V(x)$. Under what conditions, if any, is:

   Part A) The wave function $\Psi(x)$ discontinuous?

   Part B) The slope of the wave function $\frac{\partial \Psi}{\partial x}$ discontinuous?

   Part C) The curvature of the wave function $\frac{\partial^2 \Psi}{\partial x^2}$ discontinuous?

2. (30 points) In this problem we'll look at scattering off a potential with complicated structure which, as in class, we'll approximate as a series of rectangular barriers. In this problem, we'll try to understand if, given an incoming wave, we can just write down the solution to the wave function. We'll do this by examining a single step in the potential at $x = 0$. In general, there will be many other steps elsewhere in space, but if we can write down the solution for one arbitrary step, we could apply that to all the steps to solve the scattering problem.

   We'll consider the step at $x = 0$. We'll also assume that the energy of the particle is larger than the potential both for $x < 0$ and $x > 0$, so the wave functions can be written as $\exp(\pm ikx)$. Under these assumptions, we can write the wave function for $x < 0$ as $\Psi_l(x) = A\exp(ik_lx) + B\exp(-ik_lx)$, and the wave function for $x > 0$ is $\Psi_r(x) = C\exp(ik_rx) + D\exp(-ik_rx)$ (where l and r stand for left and right, respectively).

   Part A) What are the boundary conditions that the wave function must satisfy between A, B, C, and D at $x = 0$?

   Part B) Recall that the probability current is

   $$j = \frac{\hbar}{2mi}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \Psi\frac{\partial \Psi^*}{\partial x}\right) \tag{1}$$

   If we have a wave function that is the sum of two pieces $\Psi = \Psi_1 + \Psi_2$ show that in general the associated probability currents j, j_1, j_2 do *not* obey $j = j_1 + j_2$ (you might want to consider

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the case where $\Psi_1 = \Psi_2$).

Part C) Show that for the case $\Psi_1 = A \exp(ikx)$ and $\Psi_2 = B \exp(-ikx)$ that now the probability current of $\Psi_1 + \Psi_2$ *does* equal $j_1 + j_2$.

Part D) In steady state, the probability current in the left region should match the probability current in the right region, otherwise we'll build up probability in one region. This gives us an extra constraint between A, B, C, D. What is this constraint?

Part E) We can think of $A \exp(ikx)$ as the incoming wave that we sent towards the barrier, so our job is to determine B, C, D in terms of A. We now have three constraints (two from Part A, one from Part D) for three unknowns. Have we uniquely determined the values for B, C, D? Why or why not? You might want to consider why we used Equation 1 and not simply $\frac{\hbar}{im} \Psi^* \frac{\partial \Psi}{\partial t}$ for the probability current. Note - even if you didn't get the answer to part D, you can still answer this part based on physical/general mathematical grounds.

3. (30 points) We put a lot of effort into deriving wave functions given a potential, but it's much easier to go the other direction. Given a wave function, we can find what potential that makes this an energy eigenstate by plugging it into the time-independent Schrodinger equations $H\Psi = E\Psi$.

   Part A) If we work in dimensionless units, where $\hbar = m = 1$, show that the time-independent Schrodinger equation can be written

   $$V(x)\Psi = \left(E\Psi + \frac{1}{2} \frac{\partial^2 \Psi}{\partial x^2} \right) \tag{2}$$

   (I'm not after a long derivation here)

   Part B) Show that by adding a constant V_0 to $V(x)$, we can always set $E = 0$. Given an initial value for E and potential V, what should the value of V_0 be that makes $E = 0$? Note that after finding a potential, we can always shift the potential to a sensible offset (say, $V(\infty) = 0$) to get the natural energy value. Don't forget that Equation 2 has a copy of Ψ on the left, so you need to divide by that to get V.

   Part C) A simple wave function we could consider is $c \exp(-a|x|)$ where $|x|$ is the absolute value of x. Sketch the wave function and say what the value of the potential is at $x = 0$. Please specify if it's positive or negative.

Part D) Now work out the potential from the same wave function in Part C for x not equal to 0. If we set the potential at infinity to be zero, what is the energy of the state?

Part E) One other common function that goes to zero at large $|x|$ is a Lorentzian:

$$\Psi(x) = \frac{c}{1 + \frac{1}{2}x^2} \tag{3}$$

What is the potential that gives rise to this wave function? Please sketch the potential, and make sure to specify 1) the minimum value, 2) where $V = 0$, and 3) the limiting behavior of V for large x.

Part F) You should have found that if we set $E = 0$ that the potential goes to 0 at large $|x|$, so this really is a zero-energy state. Given that, could this potential support a bound state (in the sense that Ψ approaches zero for large $|x|$) with a higher energy level? Explain why or why not. Note - you should still be able to answer this question based on what I have stated here even if you did not get the previous part to work.

Bonus (up to 5 points missed elsewhere): Equation 2 also serves as a uniqueness proof. Show that the *only* potential that has a Gaussian for an energy eigenstate is the simple harmonic oscillator.

4. (25 points) The carbon monoxide molecule has a permanent electric dipole because the oxygen atom pulls the electrons towards it. That means when it rotates, it will spontaneously emit photons. You'll see in a future course that a rotating molecule like this has to have integer values for the angular momentum quantum number j, and that when the CO molecule emits a photon, j decreases by one.

Part A) Much like it's convenient to work with $p^2/2m$ for the kinetic energy in quantum mechanics, the convenient form for the kinetic energy of rotation is $J^2/2I$ where J is the angular momentum and I is the moment of inertia. If you are given I for an object, what is the rotational energy in terms of I, j (the quantum number associated with J^2), and any fundamental constants you may need?

Part B) What is the change in energy when the molecule transitions between states $j + 1$ and j? Once again, give your answer in terms of j, I, and any fundamental constants.

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Part C) When a CO molecule transitions from $j = 1$ to $j = 0$, it emits a photon with frequency 115 GHz. Estimate the distance between the carbon and oxygen atoms in CO. You can treat the CO molecule as a dumbell with $I = MR^2$ where M is the total mass (in this case of the carbon and oxygen molecules), and $2R$ is the distance between the atoms. The mass of a proton is $m_p = 1.67 \times 10^{-27}$ kg, and Planck's constant $h = 2\pi\hbar = 6.626 \times 10^{-34}$ joule-seconds. The energy of a photon is $h\nu$ (not $\hbar$). You may assume oxygen has a mass of $16m_p$, and carbon has a mass of $12m_p$. Compare this to the accepted value of 1.128Å where 1Å=10^{-10} metres.

1. (15 points) Consider a wave function $\Psi(x)$ that is an energy eigenstate for some potential $V(x)$. Under what conditions, if any, is:

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Part B) The slope of the wave function $\frac{\partial \Psi}{\partial x}$ discontinuous?

Part C) The curvature of the wave function $\frac{\partial^2 \Psi}{\partial x^2}$ discontinuous?

$$\left(\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \Psi(x) = E \Psi(x)$$

A) $\Psi(x)$ always needs to be continuous if we want to represent a physical situation (ie physical $V(x)$)

B) $\frac{\partial \Psi}{\partial x}$ is discontinuous at the boundaries of $V(x)$ when $\Psi(x)$ is not in an allowed energy state

c) from the schrödinger eqn, $\frac{d^2 \Psi}{dx^2}$ can be discontinuous if $V(x)$ is discontinuous

2. (30 points) In this problem we'll look at scattering off a potential with complicated structure which, as in class, we'll approximate as a series of rectangular barriers. In this problem, we'll try to understand if, given an incoming wave, we can just write down the solution to the wave function. We'll do this by examining a single step in the potential at $x = 0$. In general, there will be many other steps elsewhere in space, but if we can write down the solution for one arbitrary step, we could apply that to all the steps to solve the scattering problem.

We'll consider the step at $x = 0$. We'll also assume that the energy of the particle is larger than the potential both for $x < 0$ and $x > 0$, so the wave functions can be written as $\exp(\pm ikx)$. Under these assumptions, we can write the wave function for $x < 0$ as $\Psi_l(x) = A\exp(ik_lx) + B\exp(-ik_lx)$, and the wave function for $x > 0$ is $\Psi_r(x) = C\exp(ik_rx) + D\exp(-ik_rx)$ (where l and r stand for left and right, respectively).

step at $x=0$, assume $E>V$ everywhere $\rightarrow e^{\pm ikx}$
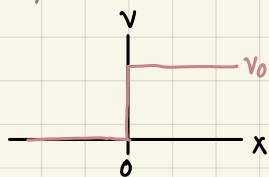
we have $\Psi(x) = \begin{cases} \Psi_l(x) = Ae^{ik_lx} + Be^{-ik_lx} & x<0 \\ \Psi_r(x) = Ce^{ik_rx} + De^{-ik_rx} & x>0 \end{cases}$

Part A) What are the boundary conditions that the wave function must satisfy between A, B, C, and D at $x = 0$?

at $x=0$, we need $\Psi(x)$ and $\frac{d\Psi(x)}{dx}$ to be continuous so we have:

$\begin{cases} A+B = C+D \\ ik_l(A-B) = ik_r(C-D) \end{cases}$

Part B) Recall that the probability current is

$$j = \frac{\hbar}{2mi}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right) \tag{1}$$

If we have a wave function that is the sum of two pieces $\Psi = \Psi_1 + \Psi_2$ show that in general the associated probability currents j, j_1, j_2 do *not* obey $j = j_1 + j_2$ (you might want to consider the case where $\Psi_1 = \Psi_2$).

① if $\Psi = \Psi_1 + \Psi_2$, then $\Psi^* = \Psi_1^* + \Psi_2^*$ and $\frac{\partial\Psi}{\partial x} = \frac{\partial\Psi_1}{\partial x} + \frac{\partial\Psi_2}{\partial x}$, $\frac{\partial\Psi^*}{\partial x} = \frac{\partial\Psi_1^*}{\partial x} + \frac{\partial\Psi_2^*}{\partial x}$

② so we have $\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x} = (\Psi_1^* + \Psi_2^*)\left(\frac{\partial\Psi_1}{\partial x} + \frac{\partial\Psi_2}{\partial x}\right) - (\Psi_1 + \Psi_2)\left(\frac{\partial\Psi_1^*}{\partial x} + \frac{\partial\Psi_2^*}{\partial x}\right)$

$= \Psi_1^*\partial_x\Psi_1 + \Psi_1^*\partial_x\Psi_2 + \Psi_2^*\partial_x\Psi_1 + \Psi_2^*\partial_x\Psi_2$

Regroup terms $\downarrow$ $-(\Psi_1\partial_x\Psi_1^* + \Psi_1\partial_x\Psi_2^* + \Psi_2\partial_x\Psi_1^* + \Psi_2\partial_x\Psi_2^*)$

$= \underbrace{(\Psi_1^*\partial_x\Psi_1 - \Psi_1\partial_x\Psi_1^*)}_{\text{from } j_1} + \underbrace{(\Psi_2^*\partial_x\Psi_2 - \Psi_2\partial_x\Psi_2^*)}_{\text{from } j_2} + \text{cross terms that don't cancel out}$

so we have $j = j_1 + j_2 + \text{cross terms}$ (where $j_n = \frac{\hbar}{2mi}(\Psi_n^*\partial_x\Psi_n - \Psi_n\partial_x\Psi_n^*)$)

if $\Psi_1 = Ae^{ikx}$ and $\Psi_2 = Be^{-ikx}$, then we have...

① $\Psi_1^* = A^* e^{-ikx}$, $\Psi_2^* = B^* e^{ikx}$

② $\partial_x \Psi_1 = Aike^{ikx}$ $\qquad$ $\partial_x \Psi_2 = -Bike^{-ikx}$
$\quad$ $\partial_x \Psi_1^* = -A^* ike^{-ikx}$ $\qquad$ $\partial_x \Psi_2^* = B^* ike^{ikx}$

③ Ignoring the $\frac{\hbar}{2mi}$ factor to keep notation simpler, the extra cross terms as shown in B)
are

$\qquad \Psi_1^* \partial_x \Psi_2 + \Psi_2^* \partial_x \Psi_1 - \Psi_1 \partial_x \Psi_2^* - \Psi_2 \partial_x \Psi_1^*$

$\qquad = A^* e^{-ikx}(-Bike^{-ikx}) + B^* e^{ikx} Aike^{ikx} - Ae^{ikx} B^* ike^{ikx} - Be^{-ikx}(-A^* ike^{-ikx})$

$\qquad = -A^* Bike^{-2ikx} + AB^* ike^{2ikx} - AB^* ike^{2ikx} + A^* Bike^{-2ikx}$

$\qquad = 0$

so we have $j = j_1 + j_2 + \overset{0}{\cancel{\text{cross terms}}}$

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we need $j_\ell = j_r$ $\Longleftrightarrow$ $\frac{\hbar k_\ell}{m}(|A|^2 - |B|^2) = \frac{\hbar k_r}{m}(|C|^2 - |D|^2)$

$\qquad\qquad\qquad k_\ell(|A|^2 - |B|^2) = k_r(|C|^2 - |D|^2)$

using def. of j,
not showing all the
steps. we did it in class...
(similar to prev. parts)

Part E) We can think of $A\exp(ikx)$ as the incoming wave that we sent towards the barrier, so our job is to determine B, C, D in terms of A. We now have three constraints (two from Part A, one from Part D) for three unknowns. Have we uniquely determined the values for B, C, D? Why or why not? You might want to consider why we used Equation 1 and not simply $\frac{\hbar}{im} \Psi^* \frac{\partial \Psi}{\partial t}$ for the probability current. Note - even if you didn't get the answer to part D, you can still answer this part based on physical/general mathematical grounds.

we have enough conditions to constrain the values of B,C,D uniquely (as soon as A is fixed), i.e. no degrees of freedom. This makes sense because the conditions arise from requiring a physical situation and conservation laws

3. (30 points) We put a lot of effort into deriving wave functions given a potential, but it's much easier to go the other direction. Given a wave function, we can find what potential that makes this an energy eigenstate by plugging it into the time-independent Schrodinger equations $H\Psi = E\Psi$.

Part A) If we work in dimensionless units, where $\hbar = m = 1$, show that the time-independent Schrodinger equation can be written

$$V(x)\Psi = \left(E\Psi + \frac{1}{2}\frac{\partial^2\Psi}{\partial x^2}\right) \qquad (2)$$

(I'm not after a long derivation here)

shrödinger equation: $\left(\frac{-\hbar}{2m}\frac{d^2}{dx^2} + V(x)\right)\Psi(x) = E\Psi(x)$

$$-\frac{1}{2}\partial_x^2\Psi(x) + V(x)\Psi(x) = E\Psi(x)$$

$$V(x)\Psi(x) = E\Psi(x) + \frac{1}{2}\partial_x^2\Psi(x)$$

Part B) Show that by adding a constant V_0 to $V(x)$, we can always set $E = 0$. Given an initial value for E and potential V, what should the value of V_0 be that makes $E = 0$? Note that after finding a potential, we can always shift the potential to a sensible offset (say, $V(\infty) = 0$) to get the natural energy value. Don't forget that Equation 2 has a copy of Ψ on the left, so you need to divide by that to get V.

① $V(x) \longrightarrow V(x) + V_0 = V'(x)$ and we want $E' = 0$

② eqn becomes $V'(x)\Psi(x) = E'\Psi(x) + \frac{1}{2}\partial_x^2\Psi(x)$

$$V(x)\Psi(x) + V_0\Psi(x) = E'\Psi(x) + \frac{1}{2}\partial_x^2\Psi(x)$$

$\downarrow V(x)\Psi(x) - \frac{1}{2}\partial_x^2\Psi(x) = E\Psi(x)$
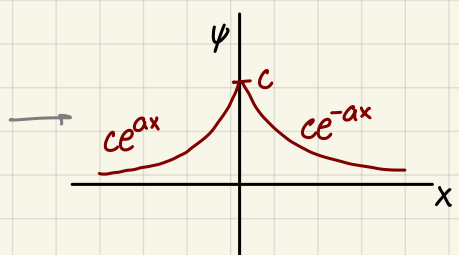
$$E\Psi(x) + V_0\Psi(x) = E'\Psi(x)$$
$$E' = E + V_0$$

$\Rightarrow E' = 0 = E + V_0$

$V_0 = -E$

Part C) A simple wave function we could consider is $c\exp(-a|x|)$ where $|x|$ is the absolute value of x. Sketch the wave function and say what the value of the potential is at $x = 0$. Please specify if it's positive or negative.

① $\Psi(x) = ce^{-a|x|} = \begin{cases} c & x = 0 \\ ce^{-ax} & x > 0 \\ ce^{ax} & x < 0 \end{cases}$

② $V(x) = E + \frac{1}{2\Psi(x)}\partial_x^2\Psi(x)$

$V(0) = E + \frac{1}{2\Psi(0)}\partial_x^2\Psi(x)|_0 \longrightarrow$ positive for large enough E

① we have $\partial_x \Psi(x) = \begin{cases} -ace^{-ax} & x>0 \\ ace^{ax} & x<0 \end{cases}$ and $\partial_x^2 \Psi(x) = \begin{cases} a^2ce^{-ax} & x>0 \\ a^2ce^{ax} & x<0 \end{cases}$

② $V(x) = E + \frac{1}{2\Psi(x)} \partial_x^2 \Psi(x)$

$= \begin{cases} E + \frac{1}{2c}e^{ax} \cdot a^2ce^{-ax} & x>0 \\ E + \frac{1}{2c}e^{-ax} \cdot a^2ce^{ax} & x<0 \end{cases}$

$V = E + \frac{a^2}{2} \quad x \neq 0$

③ since V is indep. of x (for $x \neq 0$), $V(\infty) = 0$ means that we need

$V = E + \frac{a^2}{2} = 0$

$E = -\frac{a^2}{2}$

Part E) One other common function that goes to zero at large $|x|$ is a Lorentzian:

$$\Psi(x) = \frac{c}{1 + \frac{1}{2}x^2} \tag{3}$$

What is the potential that gives rise to this wave function? Please sketch the potential, and make sure to specify 1) the minimum value, 2) where $V = 0$, and 3) the limiting behavior of V for large x.

① $\Psi(x) = c\left(1+\frac{1}{2}x^2\right)^{-1}$

$\partial_x\Psi = -c\left(1+\frac{1}{2}x^2\right)^{-2}x$

$\partial_x^2\Psi = 2c\left(1+\frac{1}{2}x^2\right)^{-3}x^2 - c\left(1+\frac{1}{2}x^2\right)^{-2}$

② $V(x) = E + \frac{1}{2\Psi(x)}\partial_x^2\Psi(x)$

$= E + \frac{1}{2c}\left(1+\frac{1}{2}x^2\right)\cdot\left[2cx^2\left(1+\frac{1}{2}x^2\right)^{-3} - c\left(1+\frac{1}{2}x^2\right)^{-2}\right]$

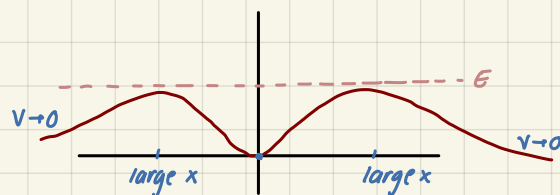$V(x) = E + x^2\left(1+\frac{1}{2}x^2\right)^{-2} - \frac{1}{2}\left(1+\frac{1}{2}x^2\right)^{-1}$

③ min $V = \frac{d}{dx}V = 0$

④ Sketch:

looking at the form of $V(x)$, $\frac{dV}{dx}$ will just be some function with powers of x so $=0$ when $x=0$
$\Rightarrow V(0) = 0$ (min & where $V=0$)

for large x, $V(x) \sim E + \frac{1}{x^2} \sim E$
and we also know $V(\infty) = 0$ since $\Psi(x)$ decays

Part F) You should have found that if we set $E = 0$ that the potential goes to 0 at large $|x|$, so this really is a zero-energy state. Given that, could this potential support a bound state (in the sense that Ψ approaches zero for large $|x|$) with a higher energy level? Explain why or why not. Note - you should still be able to answer this question based on what I have stated here even if you did not get the previous part to work.

① if $E = 0$, then $\Psi(x \text{ large}) \sim E = 0$ ✓

indep. of E

② if we have a higher energy level, then $E \neq 0$, however $V(x)$ still goes to 0 at inf. so we have regions where $E > V$ (for large enough x), ie unbound state
=> can't support a bound state for higher energies

4. (25 points) The carbon monoxide molecule has a permanent electric dipole because the oxygen atom pulls the electrons towards it. That means when it rotates, it will spontaneously emit photons. You'll see in a future course that a rotating molecule like this has to have integer values for the angular momentum quantum number j, and that when the CO molecule emits a photon, j decreases by one.

Part A) Much like it's convenient to work with $p^2/2m$ for the kinetic energy in quantum mechanics, the convenient form for the kinetic energy of rotation is $J^2/2I$ where J is the angular momentum and I is the moment of inertia. If you are given I for an object, what is the rotational energy in terms of I, j (the quantum number associated with J^2), and any fundamental constants you may need?

we know $J^2 = \hbar^2 j(j+1)$ so $E_{rot} = \dfrac{J^2}{2I} = \dfrac{\hbar^2 j(j+1)}{2I}$

Part B) What is the change in energy when the molecule transitions between states $j+1$ and j? Once again, give your answer in terms of j, I, and any fundamental constants.

① $E_j = \dfrac{\hbar^2 j(j+1)}{2I}$ and $E_{j+1} = \dfrac{\hbar^2 (j+1)(j+2)}{2I}$

② $\Delta E = E_{j+1} - E_j$

$= \dfrac{\hbar^2}{2I} \left[j(j+1) - (j+1)(j+2) \right]$

$= \dfrac{\hbar^2}{2I} (j^2 + j - j^2 - 2j - j + 2)$

$\Delta E = \dfrac{\hbar^2}{I} (1 - j)$ ⟵ lowest level in transition

Part C) When a CO molecule transitions from $j = 1$ to $j = 0$, it emits a photon with frequency 115 GHz. Estimate the distance between the carbon and oxygen atoms in CO. You can treat the CO molecule as a dumbell with $I = MR^2$ where M is the total mass (in this case of the carbon and oxygen molecules), and $2R$ is the distance between the atoms. The mass of a proton is $m_p = 1.67 \times 10^{-27}$ kg, and Planck's constant $h = 2\pi\hbar = 6.626 \times 10^{-34}$ joule-seconds. The energy of a photon is $h\nu$ (not $\hbar$). You may assume oxygen has a mass of $16m_p$, and carbon has a mass of $12m_p$. Compare this to the accepted value of 1.128Å where 1Å$=10^{-10}$ metres.

① $j = 1 \rightarrow j = 0$, GHz$= 10^9$ Hz

$\nu = 115$ GHz $\rightarrow \Delta E = h\nu$

$I = MR^2$, $M = m_c + m_o = (12 + 16)m_p$

$\rightarrow 2R = ?$

$\hbar = \dfrac{h}{2\pi}$

$m_p = 1.67 \times 10^{-27}$ kg

$h = 6.626 \times 10^{-34}$ JS

② $\Delta E = \dfrac{\hbar^2}{I} (1 - j)$ ⟵ $j = 0$ since lowest level

$h\nu = \hbar^2 \cdot \dfrac{1}{MR^2}$

$R^2 = \dfrac{h^2}{4\pi^2} \cdot \dfrac{1}{28m_p} \cdot \dfrac{1}{h(115 \text{ GHz})}$

$R = \left(\dfrac{h}{4\pi^2 \cdot 28m_p \cdot 115 \times 10^9 \text{ Hz}} \right)^{1/2}$

$2R = \left(\dfrac{h}{\pi^2 \cdot 28m_p \cdot 115 \times 10^9 \text{ Hz}} \right)^{1/2}$ ⟵ $2\sqrt{} = \sqrt{4\cdots}$

$2R = 1.117 \times 10^{-10}$ m

$2R = 1.117$ Å

very close to the accepted 1.128 Å !