Solutions to Test 3
November 8, 2004

This test consists of three parts. Please note that in parts II and III, you can skip one question of those offered.

Part I: Multiple Choice [20 points]
For each question, choose the best answer (2 points each)

1. Suppose I were to measure the total internal angular momentum (spin) of a single electron, $\vec{S}^2$. What value would I get?
   A) $\frac{1}{2}\hbar$
   B) $\frac{1}{4}\hbar^2$
   C) $\frac{3}{4}\hbar^2$ ← This one is the answer
   D) It depends on the spin of that particular electron. It is different for different electrons.
   E) It depends on what shell and subshell it is in. It is different for different electrons.

2. Under what circumstances can one use the time-independent Schrödinger equation?
   A) Only when the potential V is independent of both space and time
   B) Only when the potential V is independent of space, though it may depend on time
   C) Only when the potential V is independent of time, though it may depend on space
   D) Only on Sundays and holidays
   E) The time-independent Schrödinger equation can always be used

3. What about the Hydrogen atom problem allowed us to break the problem into a radial part and an angular part?
   A) Because we knew all the hydrogen atom wave functions would be spherically symmetric
   B) Because the hydrogen atom has an inverse square law force
   C) Because the proton is approximately spherical
   D) Because the electron is moving much slower than the speed of light
   E) Because the potential depends only on the distance r, not on θ and ϕ.

4. If I measure the expectation value of the Hamiltonian, the result will give me the expectation value of the
   A) momentum
   B) total energy
   C) kinetic energy
   D) potential energy
   E) total angular momentum

5. Which operator, in quantum mechanics, is proportional to $\partial/\partial x$?
   A) x, the position operator
   B) p, the momentum operator
   C) Δx, the uncertainty in the position
   D) H, the Hamiltonian
   E) L_z, the z-component of the angular momentum

6. A 5d electron in hydrogen has
   A) $n = 5$ and $m = 3$
   B) $n = 5$ and $m = 4$
   C) $l = 5$ and $m = 3$
   D) $n = 5$ and $l = 4$
   E) $n = 5$ and $l = 3$
   F) $n = 5$ and $l = 2$ ← None of the answers given were correct

7. What does the magnetic quantum number m (or m_l) tell you?
   A) The angular momentum around the z-axis, L_z
   B) The total angular momentum, $\vec{L}^2$
   C) The internal angular momentum (spin) around the z-axis, S_z
   D) The total internal angular momentum, $\vec{S}^2$
   E) The energy E.

8. How many electrons fit into the 2p subshell of hydrogen?
   A) One
   B) Three
   C) Five
   D) Six
   E) None of the above

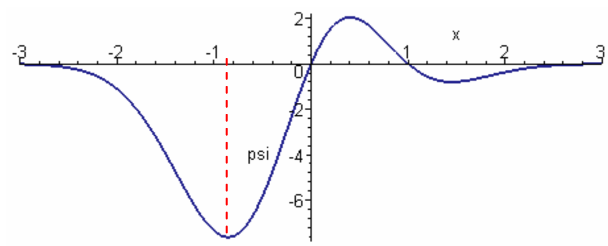
9. If you put an electron in an infinite square well, which of the following is <u>not</u> true?
   A) There is a pressure associated with this confinement, even if the temperature is zero
   B) The wave function must be continuous at the two boundaries of the square well
   C) The energy of the electron comes from the electric repulsion of the walls acting on the electron
   D) The energy of the ground state is greater than zero
   E) Light particles, like electrons, have more energy than heavy particles, like neutrons, in the same quantum state

10. What is the minimum energy of the harmonic oscillator (formulas are at the start of part III, below)?
    A) $-\hbar\omega$
    B) $-\frac{1}{2}\hbar\omega$
    C) 0
    D) $\frac{1}{2}\hbar\omega$ **← This one is the answer**
    E) $\hbar\omega$

Part II: Short answer [20 points]

Choose **two** of the following questions and give a short answer (1-3 sentences) (10 points each).

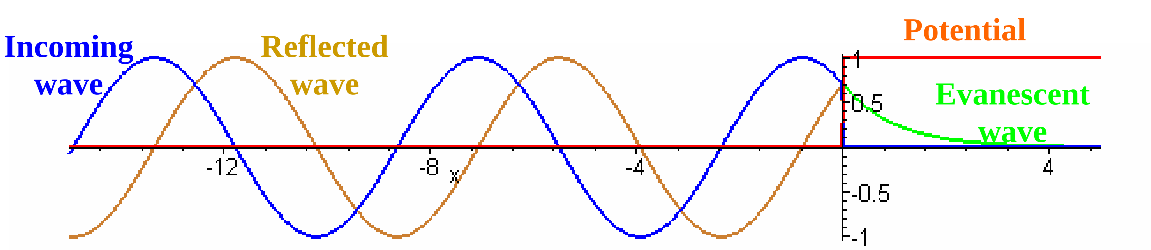
11. Plotted at right is a wave function. What is the least likely place(s) to find the particle, and what is the most likely place(s) to find the particle?



The least likely places to find the particle are where wave function vanishes, which is at $x = 0$ and $x = 1$. The most likely places are where the square is as large as possible, which is when the wave function itself is most positive or most negative. This is clearly somewhere around $x = -0.85$.

12. Give a qualitative description, possibly including a diagram, of what happens when an electron of energy $E < V_0$ encounters a step of height V_0 potential. In particular, tell me what the wave function looks like to the right of the step.

The wave function is completely reflected in this case, so there is an incoming wave on the left moving to the right, and there is a reflected wave on the left moving to the left. Inside the step there is an exponentially damped wave (the evanescent wave) that quickly falls to zero. Though I'm having a little trouble getting Maple to do what I want, the sketch below probably gives you some idea of what is going on.



13. Give a list of the four quantum numbers that completely describe an electron in hydrogen (just the letters is fine), and give me a list of restrictions on these numbers.

The four quantum numbers are called *n*, *l*, *m* (or m_l), and m_s. The restrictions are:

$$
\begin{aligned}
n &= 1, 2, 3, \ldots \\
l &= 0, 1, \ldots, n-1 \\
m &= -l, -l+1, \ldots, l-1, l \\
m_s &= \pm\tfrac{1}{2}
\end{aligned}
$$

Part III: Calculation: [60 points]

Choose **three** of the following four questions and perform the indicated calculations (20 points each). You may find the following formulas helpful:

$$\hbar = 1.055\times10^{-34}\ \text{J}\cdot\text{s} = 6.582\times10^{-16}\ \text{eV}\cdot\text{s} \qquad \alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right) \qquad E_n = \frac{\pi^2\hbar^2 n^2}{2mL^2} \qquad T \approx 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)\exp(-2\alpha L)$$

14. An electron of mass m = 9.109×10^{-31} kg has kinetic energy E = 1.000×10^{-19} J and is impacting on a barrier that is V_0 = 2.000×10^{-19} J high and 1.00 nm thick. What is the probability that the electron makes it out to the other side? Show your work.

We first need to calculate the damping coefficient α, which is given by

$$\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar} = \frac{\sqrt{2\left(9.109\times10^{-31}\ \text{kg}\right)\left(1.000\times10^{-19}\ \text{kg}\cdot\text{m}^2/\text{s}^2\right)}}{1.055\times10^{-34}\ \text{kg}\cdot\text{m}^2/\text{s}} = 4.046\times10^{9}\ \text{m}^{-1}$$

Now we simply plug this into the approximation formula for the transmission probability, which is

$$T \approx 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)\exp(-2\alpha L) = 16\cdot\frac{1}{2}\left(1-\frac{1}{2}\right)\exp\left[-2\left(4.046\times10^{9}\ \text{m}^{-1}\right)\left(1.00\times10^{-9}\ \text{m}\right)\right]$$

$$\approx 0.00122$$

15. The one-dimensional square well has potential and ground state wave functions given by

$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & \text{otherwise} \end{cases} \qquad \textbf{and} \qquad \psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$$

These waves exist only in the allowed region 0 < *x* < *L*.

(a) Show that this wave functions satisfies the time-independent Schrödinger equation, and determine the energy *E*.

The time-independent Schrödinger equation is

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

It is a little difficult to talk about the excluded region, but naïvely, you can just argue that since the wave function vanishes, this works everywhere. In the allowed region, the second term vanishes. We need two derivatives of the wave function. The derivatives are:

$$\frac{\partial}{\partial x}\psi(x) = \frac{\pi}{L}\sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{L}\right) \quad \text{and} \quad \frac{\partial^2}{\partial x^2}\psi(x) = -\frac{\pi^2}{L^2}\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)$$

Plugging these into Schrödinger's equation, we are trying to verify that

$$-\frac{\hbar^2}{2m}\left(-\frac{\pi^2}{L^2}\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\right) + 0 = E\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)$$

Canceling the sines and the square roots, this tells us that

$$E = -\frac{\pi^2\hbar^2}{2mL^2}$$

(b) Use this solution to find a solution $\Psi(x,t)$ to the time-dependent Schrödinger equation.

The general relationship between the time-dependent and time-independent solutions is

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar},$$

so in this case we have

$$\Psi(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{a}\right)e^{-iEt/\hbar} = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{a}\right)\exp\left(-\frac{i\pi^2\hbar t}{2mL^2}\right)$$

16. At the end of this problem can be found a set of possibly useful integrals. A wave function is of the form

$$\psi(x) = \frac{\sqrt{2a^3/\pi}}{x^2 + a^2}$$

(a) What is the expectation value of *x*, that is, compute $\langle x \rangle$.

This is given by

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x\psi(x)\, dx = \int_{-\infty}^{\infty} x\psi^2(x)\, dx = \int_{-\infty}^{\infty} \frac{2a^3}{\pi} \frac{x\ dx}{\left(x^2 + a^2\right)^2} = 0$$

(b) What is the expectation value of x^2, that is, compute $\langle x^2 \rangle$.

This is given by

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x^2\psi(x)\, dx = \int_{-\infty}^{\infty} x^2\psi^2(x)\, dx = \int_{-\infty}^{\infty} \frac{2a^3}{\pi} \frac{x^2\ dx}{\left(x^2 + a^2\right)^2} = \frac{2a^3}{\pi} \frac{\pi}{2a} = a^2$$

(c) What is the uncertainty in the position Δx ?

The uncertainty is given by

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = a^2 - 0^2 = a^2$$

Taking the square root, we see that $\Delta x = a$.

$$\int_{-\infty}^{\infty} \frac{dx}{x^2 + a^2} = \frac{\pi}{a} \qquad \int_{-\infty}^{\infty} \frac{xdx}{x^2 + a^2} = 0 \qquad \int_{-\infty}^{\infty} \frac{x^2dx}{x^2 + a^2} = \infty$$

$$\int_{-\infty}^{\infty} \frac{dx}{\left(x^2 + a^2\right)^2} = \frac{\pi}{2a^3} \qquad \int_{-\infty}^{\infty} \frac{xdx}{\left(x^2 + a^2\right)^2} = 0 \qquad \int_{-\infty}^{\infty} \frac{x^2dx}{\left(x^2 + a^2\right)^2} = \frac{\pi}{2a}$$

17. Listed below are some of the angular and radial wave functions for hydrogen.

(a) Write explicitly the wave function $\psi_{210}(r,\theta,\phi)$ of the electron

In general, $\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$, so we have

$$\psi_{210}(r,\theta,\phi) = R_{21}(r)Y_{10}(\theta,\phi) = \frac{r}{\sqrt{24a_0^5}}\exp\left(-\frac{r}{2a_0}\right)\sqrt{\frac{3}{4\pi}}\cos\theta = \frac{r\cos\theta}{\sqrt{32\pi a_0^5}}e^{-r/2a_0}$$

(b) What are the values of L^2, L_z, and E for this electron?

These are determined from the values $n = 2$, $l = 1$, and $m = 0$ to be

$$L^2 = \hbar^2\left(l^2 + l\right) = 2\hbar^2, \qquad L_z = m\hbar = 0, \quad \text{and} \qquad E = -\frac{13.6\text{ eV}}{n^2} = -3.40\text{ eV}$$

(c) What are the most likely angles θ compared to the z-axis where this electron is likely to be found? Recall that $0 \le \theta \le \pi$.

Examining the wave function from part (a), we see that it is proportional to $\cos\theta$, so that the probability density is given by $\cos^2\theta$. This is maximized when $\cos\theta = \pm 1$, which happens at $\theta = 0$ or $\theta = \pi$.

$$R_{10}(r) = \frac{2}{\sqrt{a_0^3}}\exp(-r/a_0) \qquad R_{20}(r) = \frac{a_0 - r/2}{\sqrt{2a_0^5}}\exp(-r/2a_0)$$

$$R_{21}(r) = \frac{r}{\sqrt{24a_0^5}}\exp(-r/2a_0)$$

$$Y_{10}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta \qquad Y_{20}(\theta,\phi) = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$$

$$Y_{21}(\theta,\phi) = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi}$$