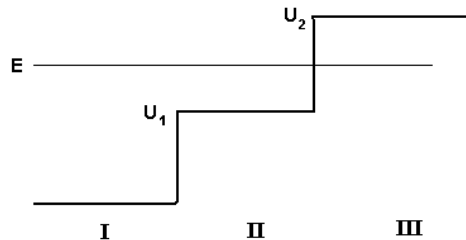


State Any Assumptions You Need To Make – Show All Work – Circle Any Final Answers
Use Your Time Wisely – Work on What You Can – Be Sure to Write Down Equations
Feel Free to Ask Any Questions

For all problems, use $c = 2.998 \times 10^8$ m/s; $h = 6.626 \times 10^{-34}$ J-s; $\hbar = 1.055 \times 10^{-34}$ J-s.

The Wall (25,000 points)

1.) Consider a plane wave in Region I heading toward the wall in the diagram shown. The energy E is in between U_1 and U_2 . From the forms of $\psi(x)$ and $\phi(t)$ given as potential solutions, write up the *form* of the solutions in Regions I, II and III. Then indicate what your B.C. (boundary conditions) would be between Regions. *Do not attempt to solve anything!*



Note: The original sketch was done by hand – but I believe this is what the picture looked like – Dr. Phil - 15 March 2004

Work, Work, Work (25,000 points)

2.) Electrons in *excited states*, those not in the ground state electronic configuration, want to get to lower energy states if they are available. (a) In the simple classically derived Bohr atom, where n is the only quantum number, all transitions are possible. List all the transitions to take an electron in the $n = 5$ state to the $n = 1$ state. *Example:* $5 \rightarrow 1$ and $5 \rightarrow 2 \rightarrow 1$. How many different paths is this?

(b) For the longest of the paths you found in (a), count up the number of degeneracies of spin-up electrons in each state. Multiplied together, this finds the total number of different combinations going from $n = 5$ state to the $n = 1$ state for a particular pathway.

(c) For the QM hydrogen atom, not all paths are possible. There are selection rules that say that $\Delta l = \pm 1$ in each step. Thus a $5s$ electron can't directly jump to the $1s$ state. There are only five allowed transitions. Use the number of degeneracies in spin-up electrons for each state and find the number of combinations for the first path listed here.

- 1.) $5s \rightarrow 4p \rightarrow 3d \rightarrow 2p \rightarrow 1s^1$
- 2.) $5s \rightarrow 4p \rightarrow 3s \rightarrow 2p \rightarrow 1s$
- 3.) $5s \rightarrow 4p \rightarrow 1s$
- 4.) $5s \rightarrow 3p \rightarrow 1s$
- 5.) $5s \rightarrow 2p \rightarrow 1s$

(d) In the real atom, there are energy differences between the levels. $4p$ and $4s$ don't have the same energy. There are now seven allowed transitions. Use the number of degeneracies in spin-up electrons for each state and find the number of combinations for the first path listed here.

- 1.) $5s \rightarrow 4p \rightarrow 4s \rightarrow 3p \rightarrow 3s \rightarrow 2p \rightarrow 1s^2$
- 2.) $5s \rightarrow 4p \rightarrow 4s \rightarrow 3p \rightarrow 1s^3$
- 3.) $5s \rightarrow 4p \rightarrow 4s \rightarrow 2p \rightarrow 1s^4$
- 4.) $5s \rightarrow 4p \rightarrow 3s \rightarrow 2p \rightarrow 1s$
- 5.) $5s \rightarrow 4p \rightarrow 1s$
- 6.) $5s \rightarrow 3p \rightarrow 3s \rightarrow 2p \rightarrow 1s^5$
- 7.) $5s \rightarrow 3p \rightarrow 1s$

¹ This transition pathway is unique to this problem, because the $3d$ state is higher than the $4s$ state in the shifted system.

² This transition pathway is unique, because the s and p states are not equal in the shifted system.

³ This transition pathway is unique, because the s and p states are not equal in the shifted system.

⁴ This transition pathway is unique, because the s and p states are not equal in the shifted system.

⁵ This transition pathway is unique, because the s and p states are not equal in the shifted system.

Bohring Atoms (25,000 points)

3.) (a) Write down the ground state electronic configuration ($1s^2 \dots$) for *iodine*.

(b) What are the four quantum numbers for the *next* electron that would be added?

Below are the functional forms of the hydrogenic atom solutions through $n = 3$.

n	l	m_l	Eigenfunction
1	0	0	$A_{100} e^{-Zr/a_0}$
2	0	0	$A_{200} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$
2	1	0	$A_{210} \left(\frac{Zr}{a_0}\right) e^{-Zr/2a_0} \cos \theta$
2	1	± 1	$A_{21\pm 1} \left(\frac{Zr}{a_0}\right) e^{-Zr/2a_0} \sin \theta e^{\pm i\phi}$
3	0	0	$A_{300} \left(27 - 18 \frac{Zr}{a_0} + 2 \frac{Z^2 r^2}{a_0^2}\right) e^{-Zr/3a_0}$
3	1	0	$A_{310} \left(6 - \frac{Zr}{a_0}\right) \frac{Zr}{a_0} e^{-Zr/3a_0} \cos \theta$
3	1	± 1	$A_{31\pm 1} \left(6 - \frac{Zr}{a_0}\right) \frac{Zr}{a_0} e^{-Zr/3a_0} \sin \theta e^{\pm i\phi}$
3	2	0	$A_{320} \frac{Z^2 r^2}{a_0^2} e^{-Zr/3a_0} (3 \cos^2 \theta - 1)$
3	2	± 1	$A_{32\pm 1} \frac{Z^2 r^2}{a_0^2} e^{-Zr/3a_0} \sin \theta \cos \theta e^{\pm i\phi}$
3	2	± 2	$A_{32\pm 2} \frac{Z^2 r^2}{a_0^2} e^{-Zr/3a_0} \sin^2 \theta e^{\pm 2i\phi}$

Source: Quantum Physics of Atoms, Molecules, Nuclei and Particles / Robert Eisberg and Robert Resnick. New York: John Wiley & Sons, 1974. aka "The Silver Bullet".

(c) Show, in any reasonable argument or fashion, that it is not possible to construct the $n = 3$ function from linear combinations of $n = 1$ and $n = 2$ functions.

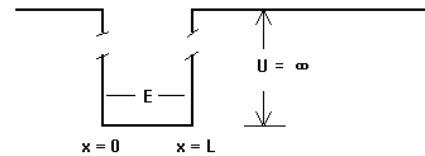
(d) From the structure of the functions for $n = 1, 2, 3$, construct the form for function $n = 8, l = 7, m_l = \pm 7, Z = 17$. Do not worry about the value of constants like 27 & 18 – we are concerned only with the terms in r, θ, ϕ , and any quantum numbers like n, l, m_l .

(e) What electron orbital is this?

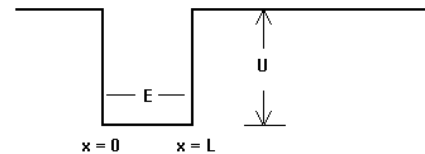
"O Schrödinger, Schrödinger, Wherefore Art Thou?" she psi'ed... (25,000 points)

4.) (a) Why do we have to square ψ^2 to see the probability, when ψ describes the whole wavefunction?

(b) For the infinite square well problem in 1-D, why did we use $\psi = A \sin(kx)$, when the general solution to the Schrödinger equation is $\psi = A \sin(kx) + B \cos(kx)$?



(c) For the finite square well problem in 1-D, where $E < U$, why do we use the general solution $\psi = A \sin(kx) + B \cos(kx)$ for the particle in the well, when we used just $\psi = A \sin(kx)$ for the infinite square well problem?



(d) Explain why we have to normalize the solution ψ .

(e) If the Schrödinger Equation is a wave equation, then what is waving?