Recitation

Atomic Structure

Q1

- **Select the best choice :**
- Most energy necessary to remove one electron:

Cu Cu^{+} Cu^{2+}

- Highest electron affinity

Cl Br I

- Greatest volume

S^{2-} Ar Ca^{2+}

R1

- **Select the best choice :**
- Most energy necessary to remove one electron:

Cu **Cu^{+}** **Cu^{2+}**

Has the greatest surplus of protons; smallest the most difficult to attract electrons from

- Highest electron affinity

Cl **Br** **I**

EA is the greatest for the smallest halogen; strongest attraction between nucleus and outermost electrons), so Cl has the highest value

- Greatest volume

S^{2-} **Ar** **Ca^{2+}**

S has the fewest protons, is therefore the largest

Q2

- Explain why Ag^{+} is the most common ion for silver.
- Which is the more likely configuration for Mn^{2+} : $[Ar]4S^{2}3d^{3}$ or $[Ar]3d^{5}$.

R2

- Ag^+ is the most common ion for silver because it has [Kr]$4d^{10}$. With filled 4d subshells ***(0.25pts)***

R1C

- The preferred configuration

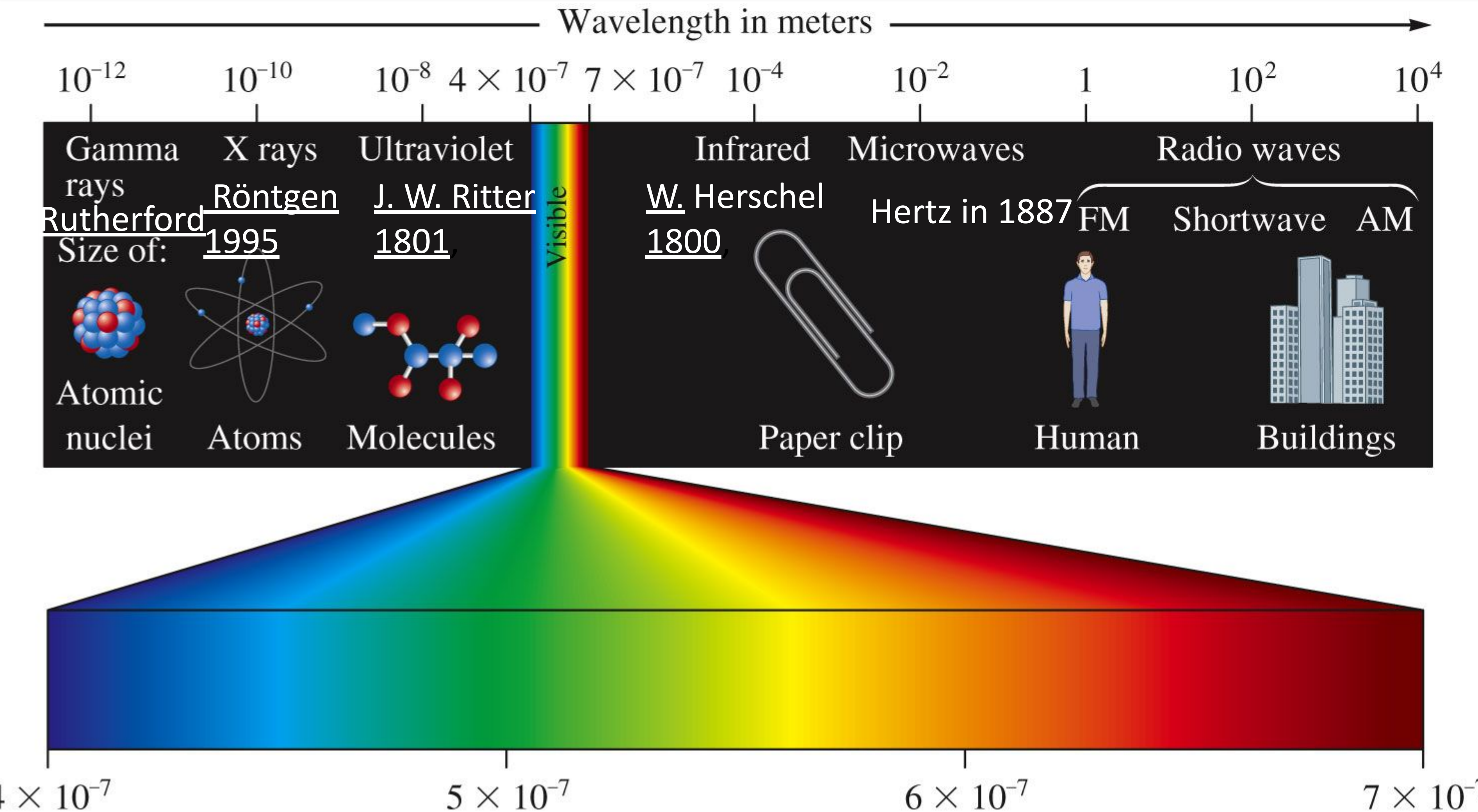
of Mn^{2+} is $[Ar]3d^5$

The 3d orbital are lower in energy than the 4s. In addition, the configuration minimizes electron-electron repulsions (because each d electron is in a separate space) and maximizes the stabilizing effect of electrons with parallel spin Πe)

3.2 Units

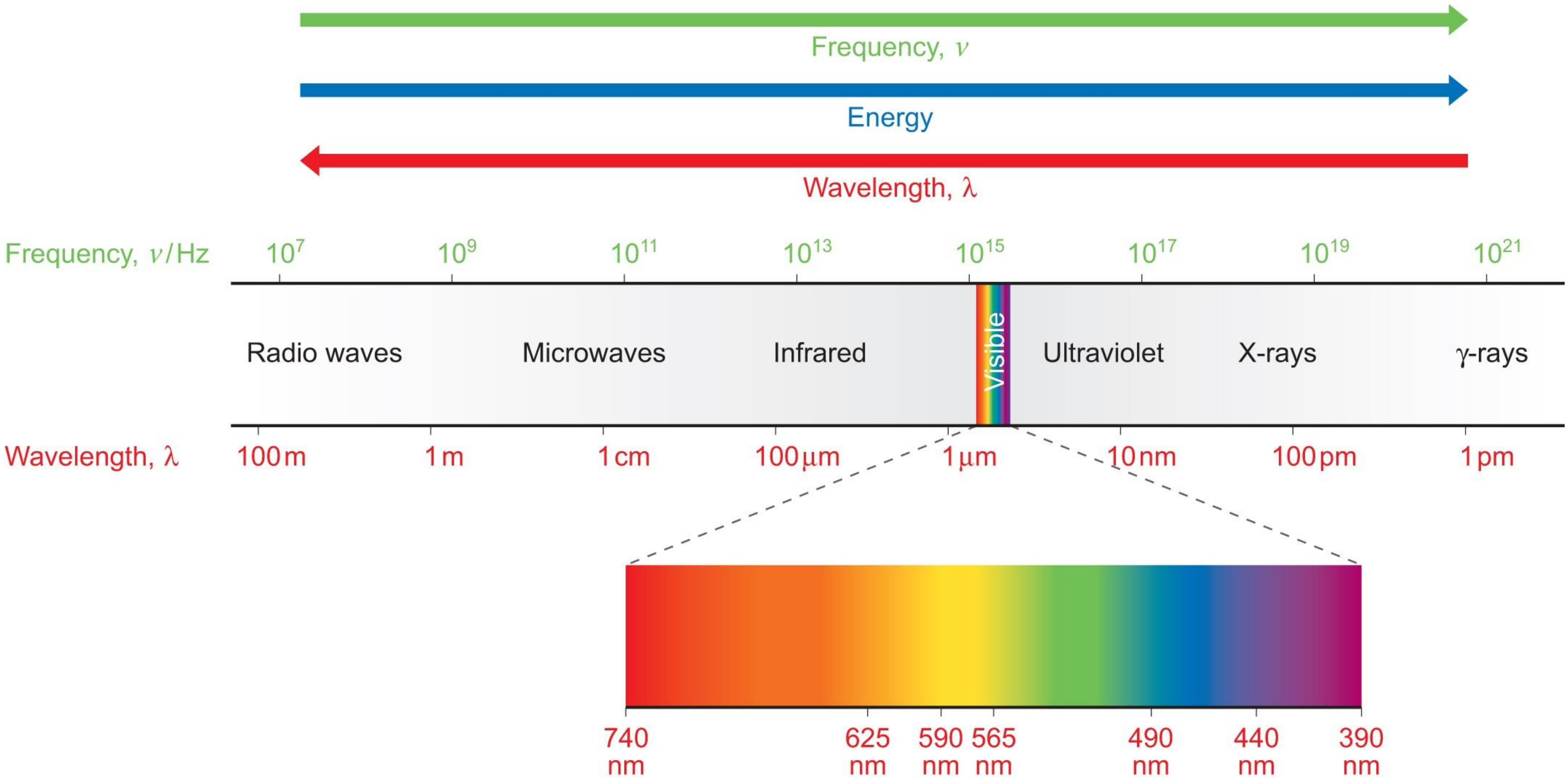
A) Electromagnetic Radiation

Spectrum

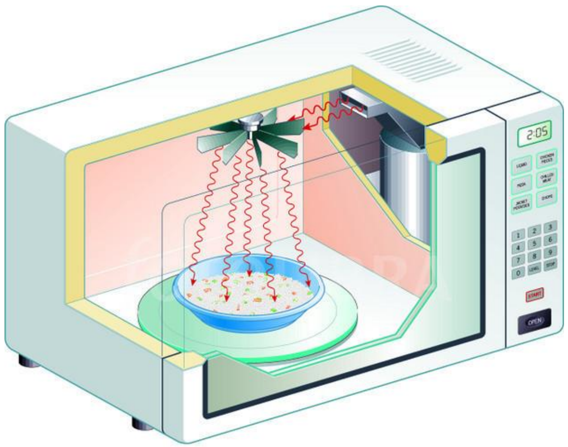


1862, Maxwell (visible and invisible are EM radiation)

ELECTROMAGNETIC RADIATION



3.2 EM Radiation



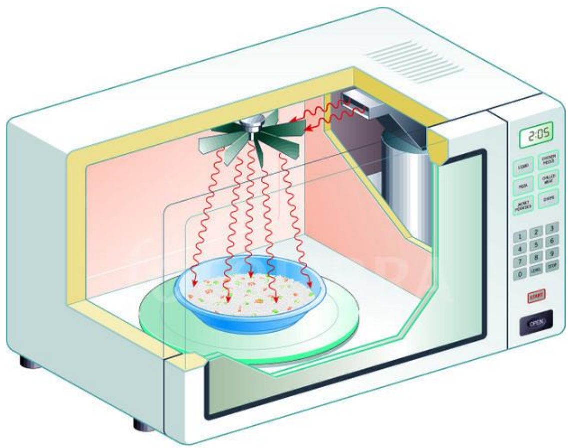
A) Electromagnetic Radiation

- The frequency of radiation used in a typical microwave oven is 1.00×10^{11} Hz. What is the energy of a mole of microwave photons with this frequency

a. 39.9 J mol^{-1}
b. 3.99 J mol^{-1}
c. 399 J mol^{-1}
d. 0.39 J mol^{-1}

3.2 Units

A) Electromagnetic Radiation



- The frequency of radiation used in a typical microwave oven is 1.00 × 1011 Hz. What is the energy of a mole of microwave photons with this frequency

h, the Planck constant = 6.626×10^{-34} J s

Avogadro constant, 6.022×10^{23} mol^{-1}

Solution 1

$E = h\nu$,

Multiply this value by the Avogadro constant to find the energy of a mole of photons (where the Avogadro constant, N_A, is the number of entities in a mole.

$E = h\nu$, to calculate the energy of one photon where

- h, the Planck constant = 6.626×10^{-34} J s
- $\nu = 1.00 \times 10^{11}$ Hz (s^{-1})
- $E = (6.626 \times 10^{-34}$ J s$) \times (1.00 \times 10^{11}$ $s^{-1})$ $E =$ 6.63×10^{-23} J

- The value for a single photon can then be converted into the energy for one mole of photons by multiplying by the Avogadro constant, 6.022×10^{23} mol^{-1}

Solution

a. 39.9 J mol^{-1}

b. 3.99 J mol^{-1}

c. 399 J mol^{-1}

d. 0.39 J mol^{-1}

3.2 Atomic Spectra

A) What is the ionization energy (kJ/mol) for an excited state of hydrogen in which the electron has already been promoted to n = 2 level?

$R_H = 3.29 \times 10^{15}$ Hz (Hz = s^{-1})

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

Avogadro Constant = 6.022×10^{23} mol^{-1}

$$\nu = R_H \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \text{ and } R_H = 3.29 \times 10^{15} \text{ Hz}$$

$$E = h\nu$$

$$E = N_A h \nu$$

3.2 Response

A

$$\nu = R_{\mathrm{H}}\left[\frac{1}{n_1^{\,2}} - \frac{1}{n_2^{\,2}}\right] \text{ and } R_{\mathrm{H}} = 3.29 \times 10^{15}\ \mathrm{Hz}$$

$n_1 = 2$ to $n_2 = \infty$ (infinity)

$$\nu = R_{\mathrm{H}}\left[\frac{1}{2^2} - \frac{1}{\infty^2}\right] = \left[\frac{1}{4} - 0\right] = 8.23 \times 10^{14}\ \mathrm{Hz}\ (\mathrm{s}^{-1})$$

3.2 Response

A

$$E = h\nu$$

$$E = (8.23 \times 10^{14}\ \mathrm{s^{-1}}) \times (6.626 \times 10^{-34}\ \mathrm{J\ s})$$

$$E = 5.45 \times 10^{-19}\ \mathrm{J}\ \text{ or }\ 5.45 \times 10^{-22}\ \mathrm{kJ}$$

$$E = N_A h\nu$$

$$E = (5.45 \times 10^{-22}\ \mathrm{kJ}) \times (6.022 \times 10^{23}\ \mathrm{mol^{-1}})$$

$$E = 328\ \mathrm{kJ\ mol^{-1}}$$

Exercise

A line from the Pfund series has the frequency 8.02×10^{13} Hz. What value of n_2 generates this line in the spectrum?

a. 5
b. 6
c. 7
d. 8

Useful Table 3.4. The atomic spectrum of hydrogen

Series	Region of the electromagnetic spectrum	n_1	n_2
Lyman	Ultraviolet	1	2, 3, 4, . . .
Balmer	Visible	2	3, 4, 5, . . .
Paschen	Infrared	3	4, 5, 6, . . .
Brackett	Infrared	4	5, 6, 7, . . .
Pfund	Infrared	5	6, 7, 8, . . .

$$\nu = R_H \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \text{ and } R_H = 3.29 \times 10^{15} \text{ Hz}$$

Exercise

A line from the Pfund series has the frequency 8.02 × 10^{13} Hz. What value of n_2 generates this line in the spectrum?

$$\frac{\nu}{R_H} = \left[\frac{1}{n_1^{\ 2}} - \frac{1}{n_2^{\ 2}}\right]$$

$$\frac{8.02 \times 10^{13}\ \text{Hz}}{3.29 \times 10^{15}\ \text{Hz}} = \left[\frac{1}{5^2} - \frac{1}{n_2^{\ 2}}\right]$$

$$0.02438 = \left[\frac{1}{25} - \frac{1}{n_2^{\ 2}}\right] = 0.04 - \frac{1}{n_2^{\ 2}}$$

Exercise

A line from the Pfund series has the frequency 8.02 × 10^{13} Hz. What value of n_2 generates this line in the spectrum?

$$\frac{\nu}{R_H} = \left[\frac{1}{n_1{}^2} - \frac{1}{n_2{}^2}\right]$$

$$\frac{8.02 \times 10^{13} \text{ Hz}}{3.29 \times 10^{15} \text{ Hz}} = \left[\frac{1}{5^2} - \frac{1}{n_2{}^2}\right]$$

$$0.02438 = \left[\frac{1}{25} - \frac{1}{n_2{}^2}\right] = 0.04 - \frac{1}{n_2{}^2}$$

Exercise

Rearranging, by taking 0.04 from each side, gives

$$-0.01563 = -\frac{1}{n_2^{\,2}}$$

Dividing both sides by –0.01563 and multiplying by n^2 gives

$$n_2^{\,2} = \frac{-1}{-0.01563} = 64$$

a. 5

b. 6

c. 7

d. 8

$n_2 = 8$

3.2 Light Interference

In Thomas Young's experiment when he passed light through two closely placed slits, it gave an interference pattern. This evidence suggests that light behaves as a particle.

True

false?

1.2 Light Interference

false?

A set of maxima and minima in an interference pattern suggests a totally different effect. As shown in Figures 3.7 and 3.8 (p.114), this experiment is demonstrating the wave like properties of light, where the interference pattern is generated from individual waves adding together (in phase) or subtracting from one another (out of phase).

Q4

The wave function of an electron is related to the probability for finding a particle in a given region of space.

$$P = \int \Psi^2 dV$$

The relationship is given by:

$$1 = \int_{all\ space} \Psi^2 dV$$

If we integrate the square of the wave function over a given volume we find the probability that the particle is in that volume. In order for this to be true the integral over all space must be one.

The volume element can be given by $= \mathbf{r^2 dr \sin\theta\, d\theta\, d\phi}$

$$v = r^2 dr \int_0^{2\pi} \int_0^{\pi} \sin\theta d\theta d\varphi = X$$

Find *X* of the integration above. Show your integration steps

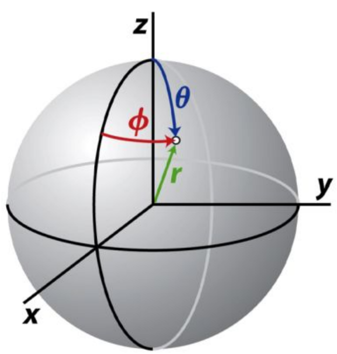
Radial Probability Distribution

The product of the three sides of the cube is equivalent to

$$r^2 \sin\theta d\theta d\varphi dr$$

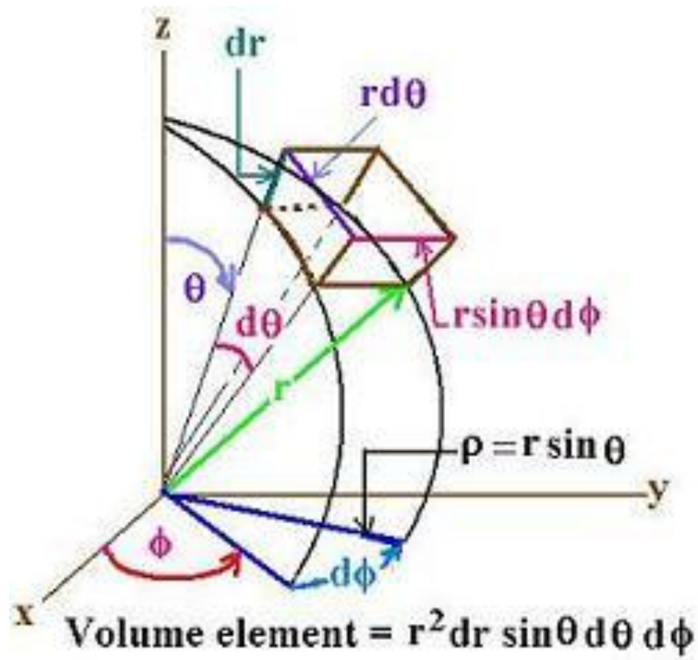
$$r^2 dr \int_0^{2\pi}\int_0^{\pi} \sin\theta d\theta d\varphi = \text{X?}$$

This integral is useful in describing the electron Density as function of distance from the nucleus



https://www.youtube.com/watch?v=Prf_jzbD_bM

$\Psi(r, \theta, \varphi)=R(r)\ Y(\theta, \varphi)$



Radial Distance

$$\boldsymbol{r^2 dr \int_0^{2\pi} \int_0^{\pi} \sin\theta d\theta d\varphi} = \text{X?}$$

$$v = r^2 dr \times -cos\theta]_0^{\pi} \times \emptyset]_0^{2\pi}$$

$$v = r^2 dr \times (-cos\pi) - (-cos0).(2\pi\text{-}0)$$

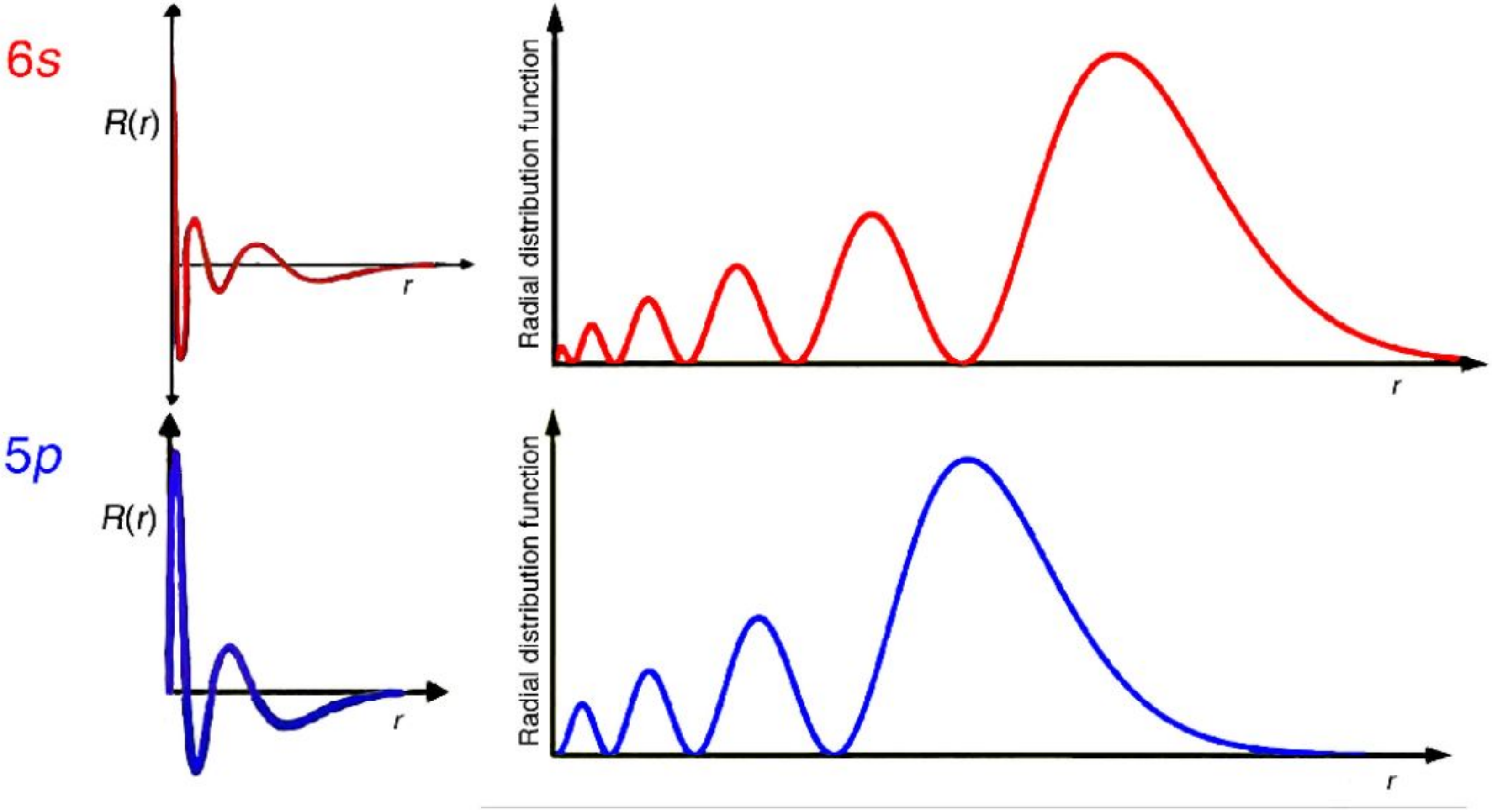
$$v = r^2 dr \times (-(-1)) - (-(1)).(2\pi\text{-}0)$$

$$v = r^2 dr \times 2.2\pi = 4\pi r^2 dr$$

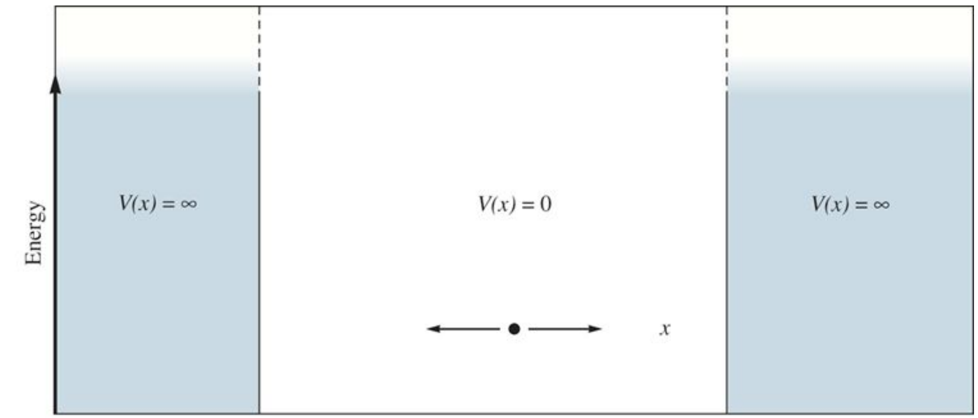
Exercise

Sketch radial wavefunctions, radial distribution functions and boundary diagrams for 6*s* and 5*p* electrons

Radial nodes for S = n-1 Radial nodes for p = n-2



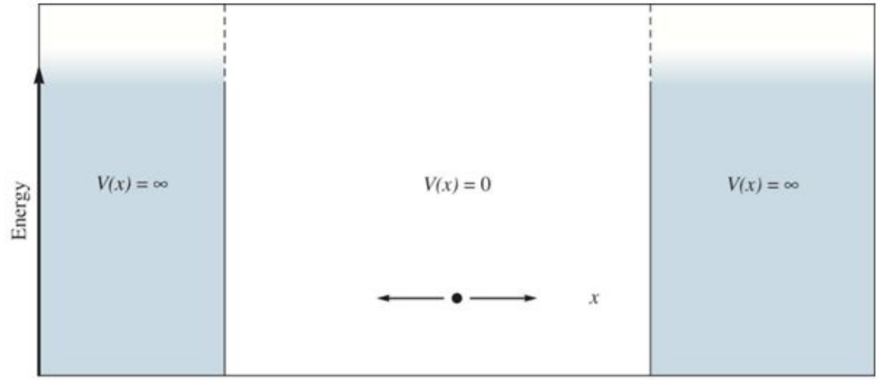
Particle in a Box



X =0 x = a

$$\frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2 \Psi(x)}{\partial x^2}\right) = E\Psi(x)$$

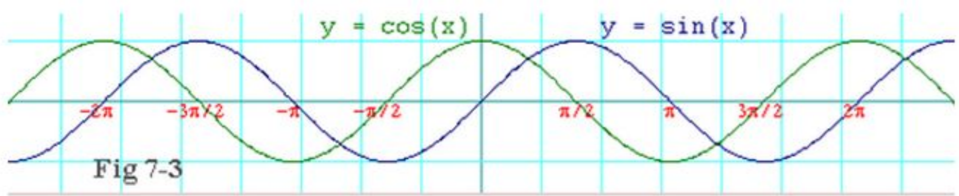
Answer 2



X =0 x = a

If $V = 0$

$$\frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2 \Psi\ (x)}{\partial x^2}\right) = E\Psi(x)$$



plots of sin(x) and cos(x)

The wave function maybe described by a combination of Sine and Cosine

Ψ = *A*sin*rx* + *B*cos *sx (A, B, r, and s are constants)*

$$\frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2 \Psi\ (x)}{\partial x^2}\right) = E\Psi(x)$$; $\Psi = A\mathrm{sin}rx + B\mathrm{cos}\ sx$

$$\frac{\partial \Psi}{\partial x} = Ar\cos rx - Bs\sin sx$$

$$\boxed{\frac{\partial^2 \Psi}{\partial x^2} = -Ar^2 \sin rx - Bs^2 \cos sx}$$

$$= \frac{h^2}{8m\pi^2}(Ar^2 \sin rx + Bs^2 \cos sx) = E\ (A \sin rx + B \cos sx)$$

If this is true, then the coefficient of the sine and cosine terms must be independently equal

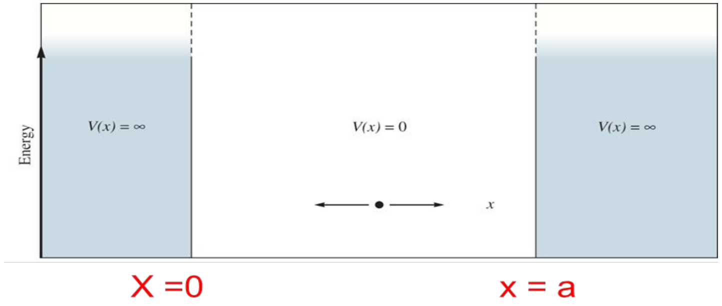
$$\frac{h^2 A r^2}{8m\pi^2} = EA, \quad \frac{h^2 B s^2}{8m\pi^2} = EB$$

$$r^2 = s^2 = \frac{8\pi^2 mE}{h^2}; r = s = \sqrt{2mE}\frac{2\pi}{h}$$

- Show that if $\Psi = A\sin rx$, the boundary conditions require that ($\Psi = 0$ when $x = 0$ and $x = a$) require that

$$r = \mp \frac{n\pi}{a}$$

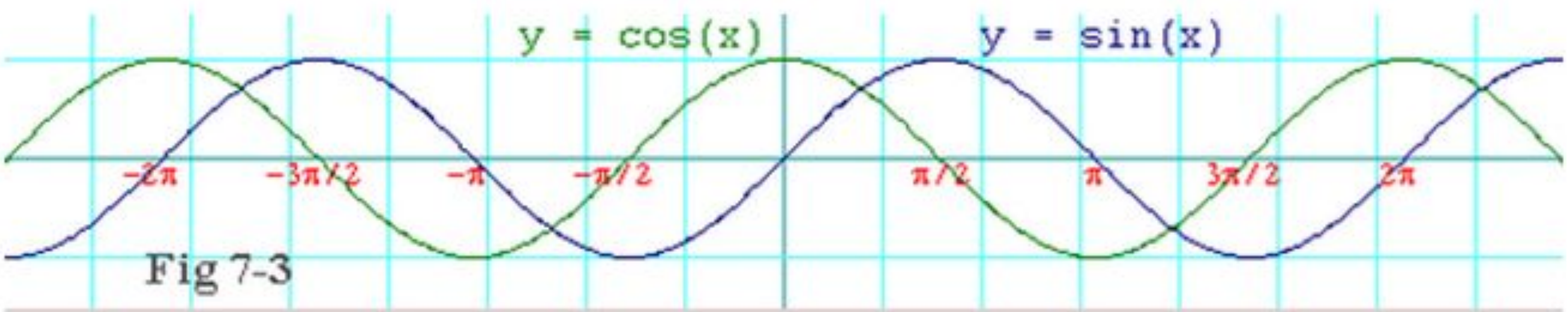
where n = any integer other than 0,



Boundary conditions : Find r

1) The particle in in the box (not outside!) = $\psi(0) = 0$ and $\psi(a) = 0$
2) The total probability to find the particle in the box = 1
3) The wave function is continuous

When $\boldsymbol{x = 0}$, $\Psi = A\sin rx = A\sin 0 = 0$



plots of sin(x) and cos(x)

- Show that if

$$r = \mp \frac{n\pi}{a}$$

, the energy levels of the particle are given by

$$E = \frac{n^2h^2}{8ma^2}$$

If $r = \mp \frac{n\pi}{a}$ $E = \frac{h^2 r^2}{8m\pi^2}$

$$E = \frac{h^2 \left(\frac{n\pi}{a}\right)^2}{8m\pi^2} = \frac{n^2\pi^2}{a^2}\frac{h^2}{8m\pi^2} = \frac{n^2 h^2}{8ma^2}$$

If we expand the solution to 3D we will get three Quantum numbers, n, l, m

- Show that substituting the value of r given in question C into $\psi = A \sin rx$ and applying the normalization requirement gives :

$$\int_0^a \psi^2(0)dx = 1 \rightarrow \int_0^a A^2 \sin^2\left(\frac{n\pi}{a}x\right)dx = 1$$

$$\int_0^a \sin^2\left(\frac{n\pi}{a}x\right)dx = \frac{1}{A^2}$$

$$\frac{a}{2} = \frac{1}{A^2} \rightarrow A = \sqrt{\frac{2}{a}}$$

$$\begin{cases} \boxed{\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)} \\ E = \dfrac{r^2\hbar^2}{2m} = \dfrac{\left(\frac{n\pi}{a}\right)\hbar^2}{2m} = \dfrac{nh^2}{8ma^2} \end{cases}$$

Integration

$$\boxed{A =} \frac{1}{\sqrt{\int_0^L \sin^2\frac{n\pi x}{L}.dx}}$$

$$\boxed{\sin^2 u = \left(\frac{1-\cos 2u}{2}\right)}$$

$$= \frac{1}{\sqrt{\int_0^L \left(\frac{1-\cos 2u}{2}\right).dx}}$$

$$\boxed{\int \cos ax.dx = \frac{1}{a}\sin ax}$$

$$= \frac{1}{\sqrt{\int_0^L \left(\frac{1}{2}\right).dx - \left(\frac{1}{2}\right)\cos 2\frac{n\pi x}{L}dx}}$$

$$\int \cos 2\frac{n\pi x}{L}dx = \frac{L}{2n\pi}\sin 2\frac{n\pi x}{L}dx$$

$$= \frac{1}{\sqrt{\left(\frac{1}{2}\right).x]_0^L - \left(\frac{1}{2}\right)\frac{L}{2n\pi}\sin 2\frac{n\pi x}{L}\Big]_0^L}}$$

$$\boxed{\begin{array}{l} \sin n\pi = 0 \\ \sin 0 = 0 \end{array}}$$

$$= \frac{1}{\sqrt{\left(\frac{L}{2}-\frac{0}{2}\right)-\left(\frac{1}{4n\pi}\right)(0-0)}} = \frac{1}{\sqrt{\left(\frac{L}{2}\right)}} = \frac{\sqrt{2}}{\sqrt{L}} = \boxed{\sqrt{\frac{2}{L}}}$$

Schrodinger Equation

What is the normalization constant for the wave function exp(-ax) over the range from 0 to infinity?

A. a
B. 2a
C. $\sqrt{a}$
D. $\sqrt{2a}$

What is the normalization constant for the wave function exp(-ax) over the range from 0 to infinity?

A. a
B. 2a
C. √a
D. √2a

$$\int_0^\infty (Ne^{-ax})^2 .\mathrm{dx} = 1$$

$$= N^2 \int_0^\infty e^{-2ax} .\mathrm{dx} = 1$$

$$\left.\frac{1}{-2a} e^{-2ax}\right]_0^\infty N^2 = -\frac{1}{2a} . 0 + \frac{1}{2a} . 1 = \frac{1}{2a}$$

$$N^2 = 2a \ = N = \ \sqrt{2a}$$

Answer-4

Match the type of orbital defined by the quantum numbers given in questions (a) to (d) in the left column, to the answers given in the right column.

a. *n* equals 2, *l* equals 3 = 4*d* orbital
b. *n* equals 4, *l* equals 2 = value of *n* not allowed
c. *n* equals 0, *l* equals 0 = 5*f* orbital
d. *n* equals 5, *l* equals 3 = value of *l* not allowed for this value of *n*

a. *n* equals 2, *l* equals 3 = 4*d* orbital (not possible) *l* must be less than *n*
b. *n* equals 4, *l* equals 2 = value of *n* not allowed
c. *n* equals 0, *l* equals 0 = 5*f* orbital (not possible) / *n* cannot be zero
d. *n* equals 5, *l* equals 3 = value of *l* not allowed for this value of *n*

Slater Rules

- Use Slater’s rules to determine the relative sizes of N, O and F atoms.

  a. F>O>N
  b. N>F>O
  c. F<O<N
  d. O>F>N

Slater Rules

- Step-1

N (Z = 7) is $1s^2 2s^2 2p^3$

O (Z = 8) is $1s^2 2s^2 2p^4$

F (Z = 9) is $1s^2 2s^2 2p^5$

- Step-2 find S

According to Slater's rules an electron in the same shell screens at 0.35, while an electron in the (n–1) shell screens at 0.85. The shielding for each is therefore

N = (4 x 0.35) + (2 x 0.85) = 2.40

O = (5 x 0.35) + (2 x 0.85) = 2.75

F = (6 x 0.35) + (2 x 0.85) = 3.10

Slater Rules

- Use Slater’s rules to determine the relative sizes of N, O and F atoms.

  a. F>O>N

  b. N>F>O

  *** c.** F<O<N

  d. O>F>N

Electronic Configuration

Q3

What are the values and quantum numbers ***l*** and ***n*** of a ***5d*** electron.

n = 5 and l = 2

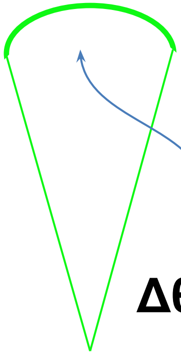
Answer 2

for any d orbitals the ***l = 2, n = 5***

n	*l*	m_l	Number of orbitals	Orbital Name	Number of electrons
1	0	0	1	1*s*	2
2	0	0	1	2*s*	2
	1	-1, 0, +1	3	2*p*	6
3	0	0	1	3*s*	2
	1	-1, 0, +1	3	3*p*	6
	2	-2, -1, 0, +1, +2	5	3*d*	10
4	0	0	1	4*s*	2
	1	-1, 0, +1	3	4*p*	6
	2	-2, -1, 0, +1, +2	5	4*d*	10
	3	-3, -2, -1, 0, +1, +2, +3	7	4*f*	14

R1c

- Explain factors that cause lanthanide contraction. ***(0.25pts)***
- Explain why Ag^+ is the most common ion for silver. ***(0.25pts)***
- Which is the more likely configuration for Mn^{2+} : $[Ar]4S^2 3d^3$ or $[Ar]3d^5$. ***(0.25pts)***



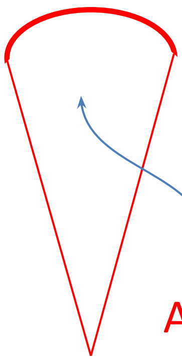
**ρsinφΔ
θ**

Δθ = $\frac{\text{Arc Length}}{\text{radius } (\rho\sin\varphi)}$

**Δ
ρ**

Angle = $\frac{\text{Arc Length}}{\text{radius of the circle}}$

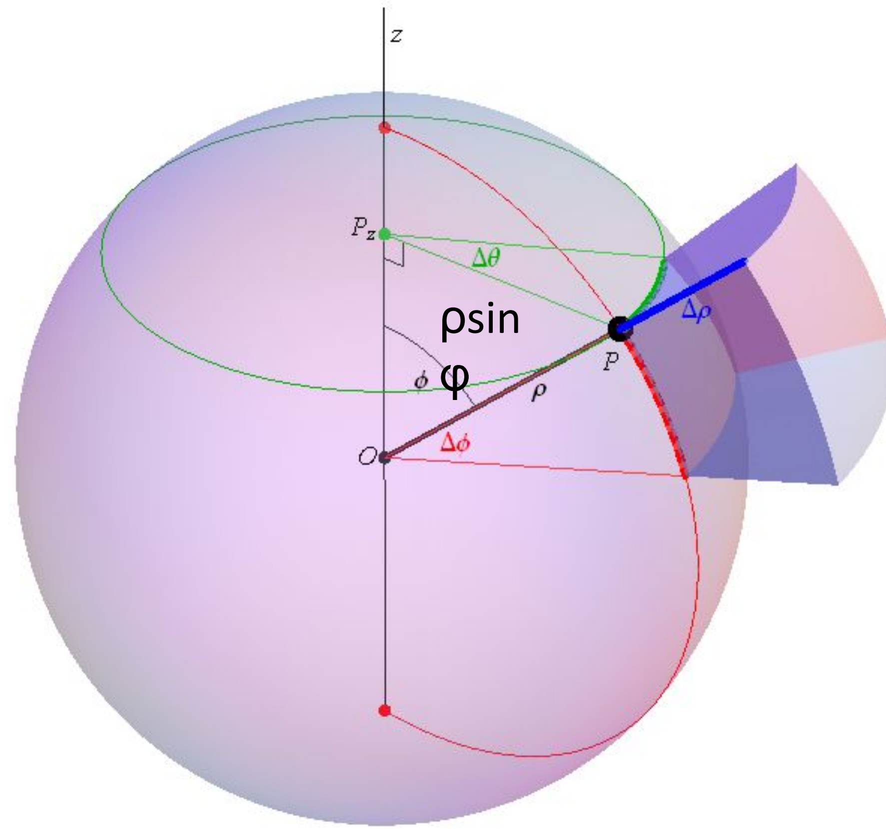
Arc Length =
ρsinφΔθ



**ρΔ
φ**

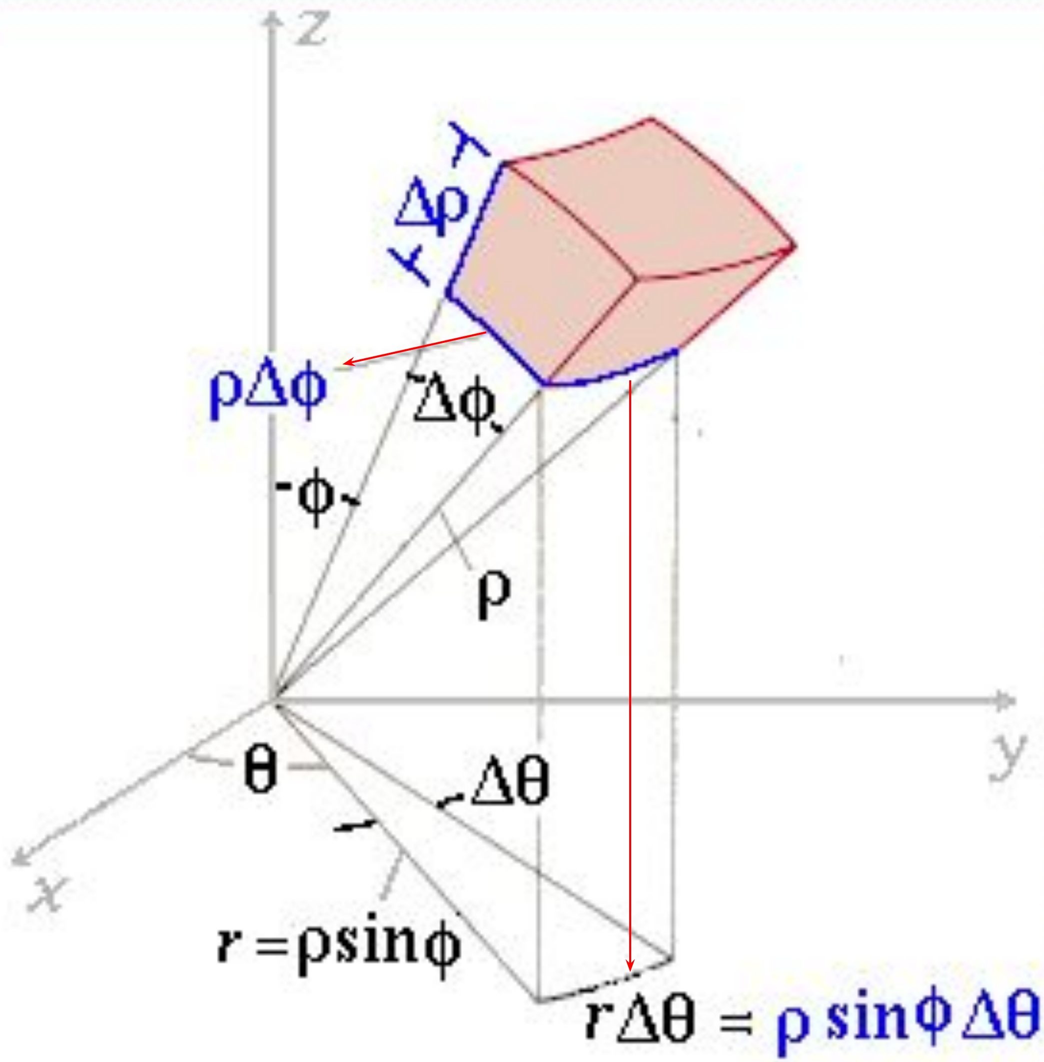
Arc Length =
ρΔφ

Δφ = $\frac{\text{Arc Length}}{\text{radius of the circle}}$



Arc Length × Arc Length × **Δρ**

**V = ρsinφ Δθ
ρΔφΔρ**



$$\Delta V = (\Delta\rho)(\rho\Delta\phi)(\rho\sin\phi\,\Delta\theta)$$

$$\Rightarrow\ dV = \rho^2 \sin\phi\, d\rho\, d\phi\, d\theta$$