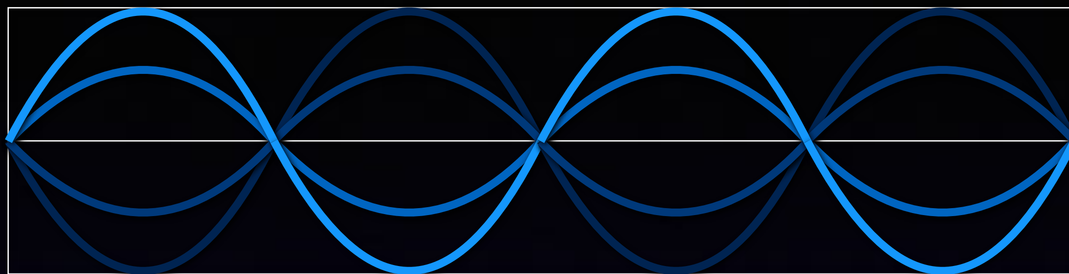
Previously in Molecularity…

Waves!



$$\psi(x,t) = A\sin\left(\frac{n\pi x}{d}\right),\ n = 4$$

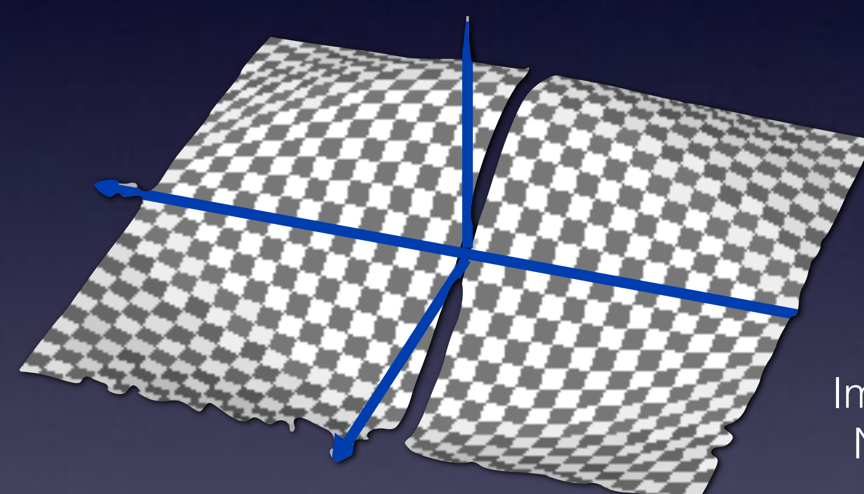
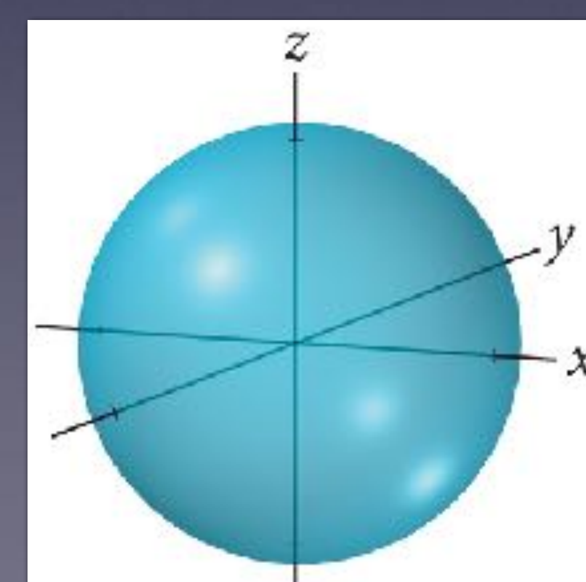


Image credit:
Nate Lewis



Tro, Fig. 7.24

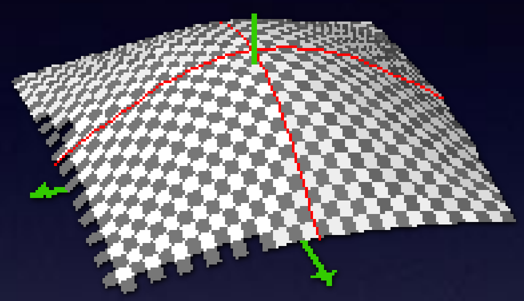
Where are we going today?

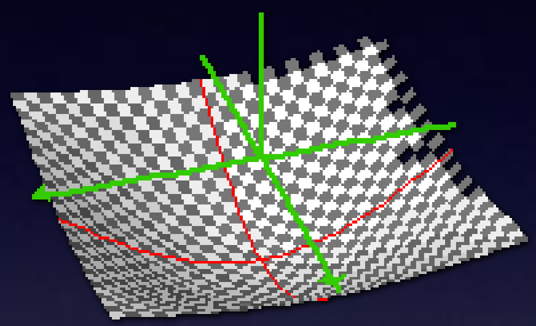
Ch1010-A17-A03 Lecture 5

- Quantistry continued!
- § 2.6 Quantum numbers
- § 2.6 Atomic orbitals:
  Shapes, sizes, smells, etc.

http://stevedeace.com/wp-content/uploads/2012/11/

Waves in two dimensions





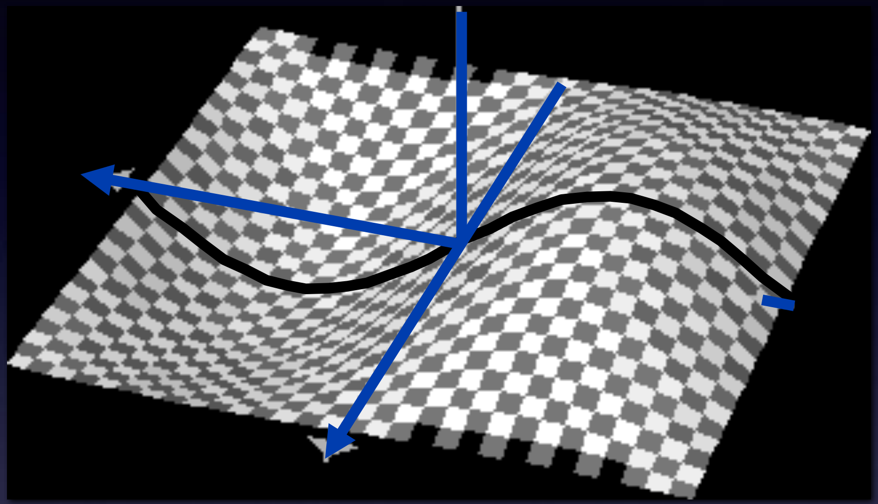
No nodes:
lowest in energy

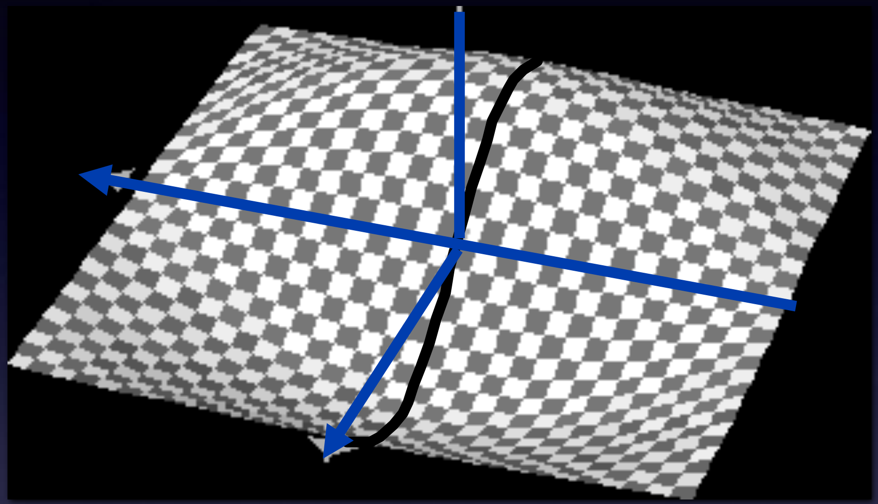
Ernst Chladni
www.hps.cam.ac.uk
chladni.jpg

In two dimensions, nodes can be radial:
https://www.youtube.com/watch?v=CGiiSIMFFII

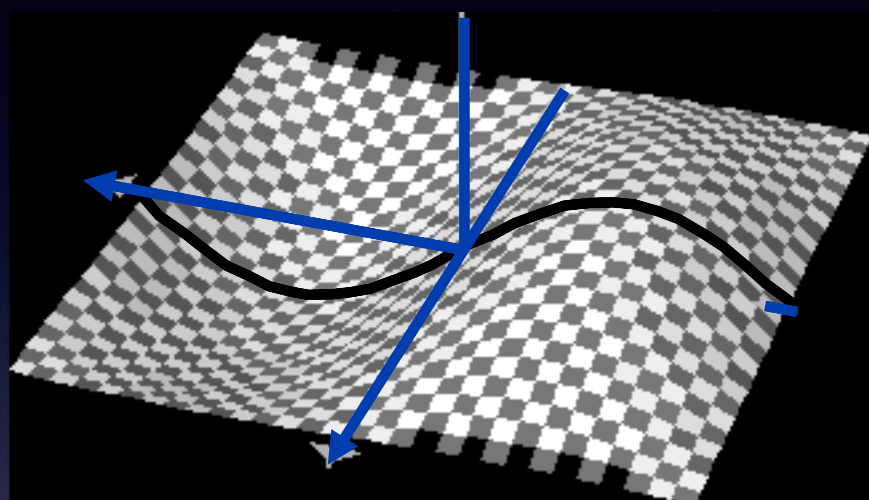
Or they can be more interesting geometries
with angular components:
https://www.youtube.com/watch?v=wMIvAsZvBiw

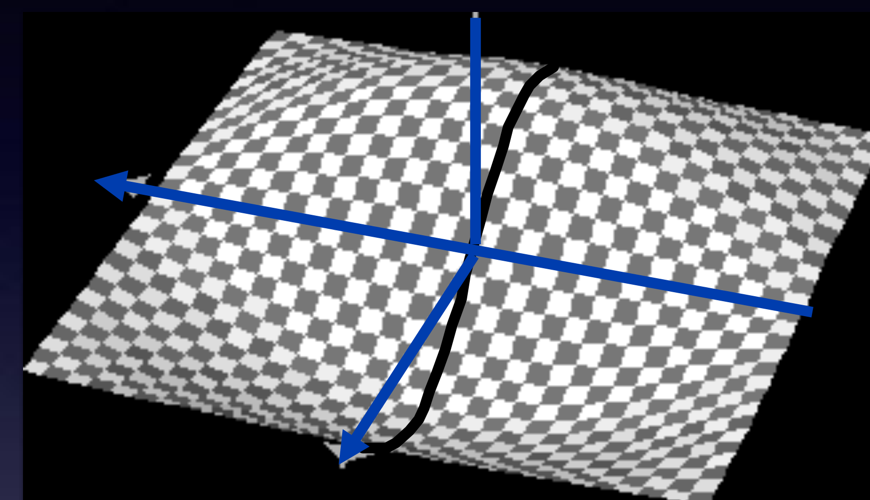
Degenerate waves

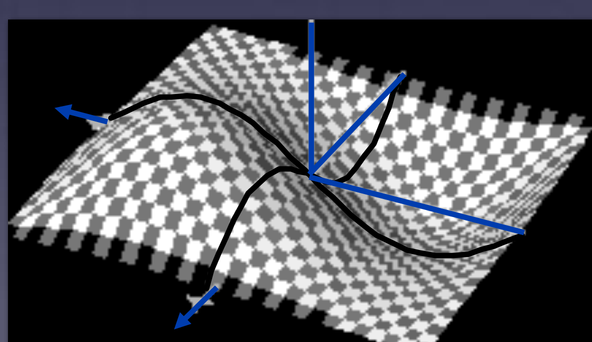




Degenerate waves







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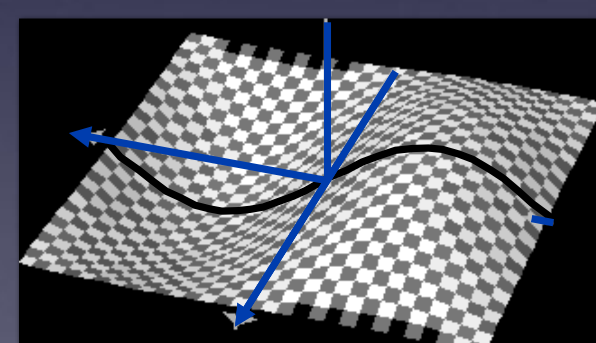

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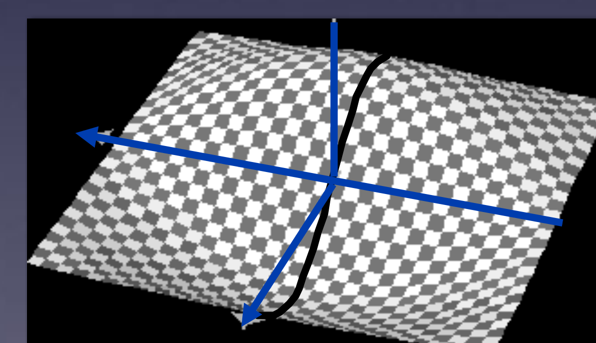
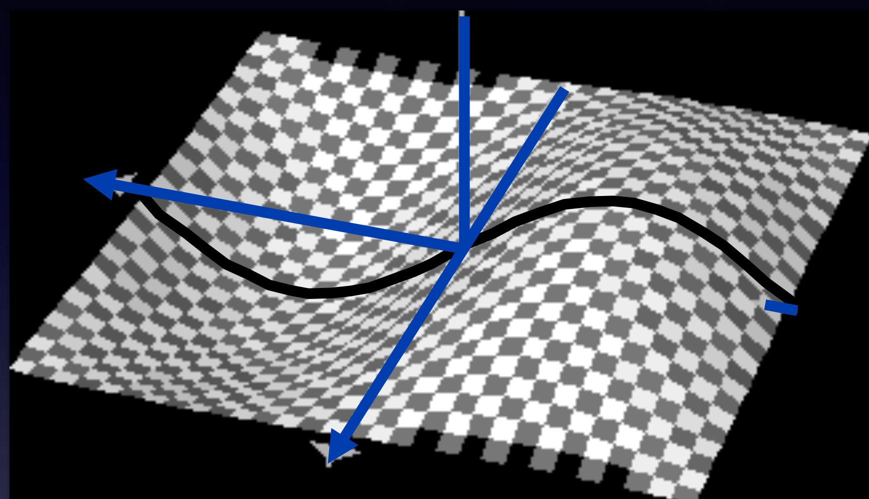
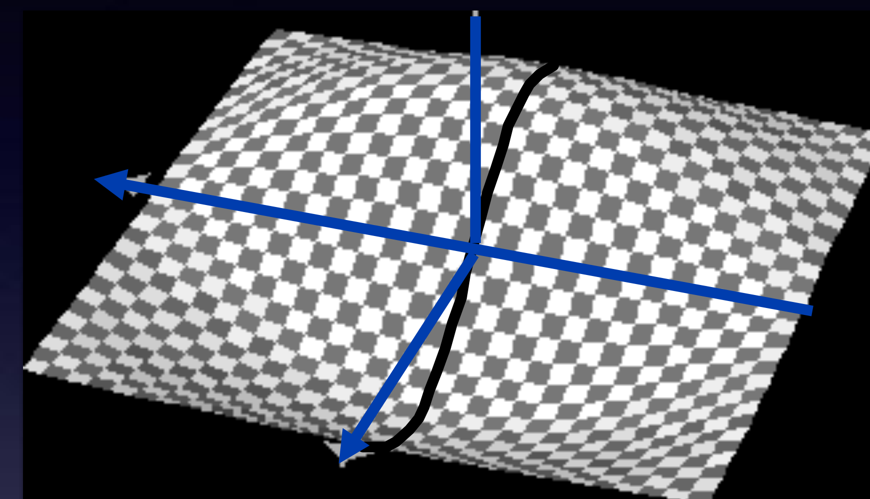
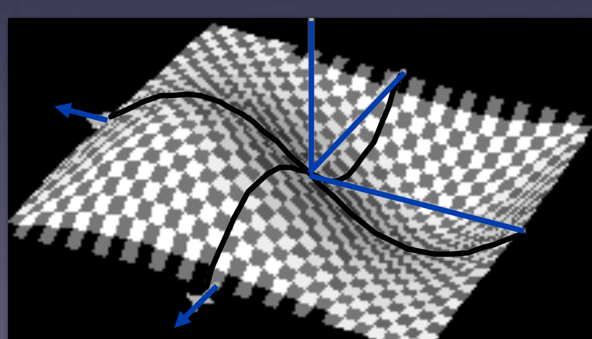
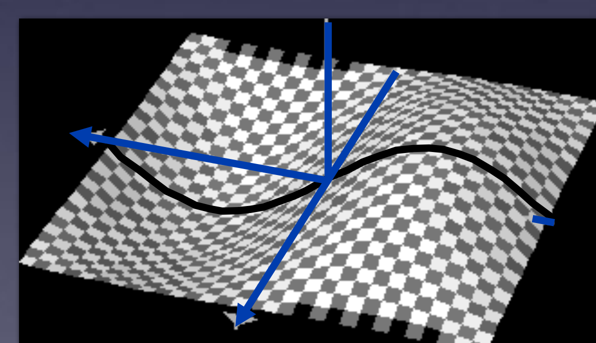
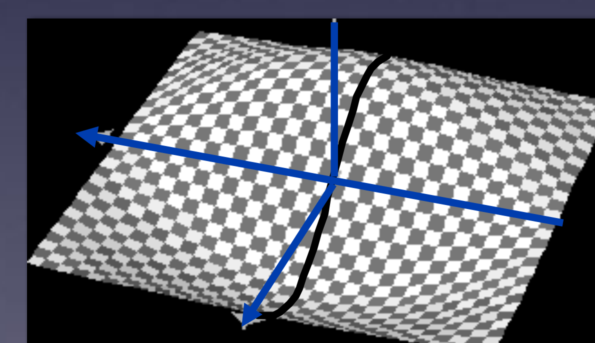
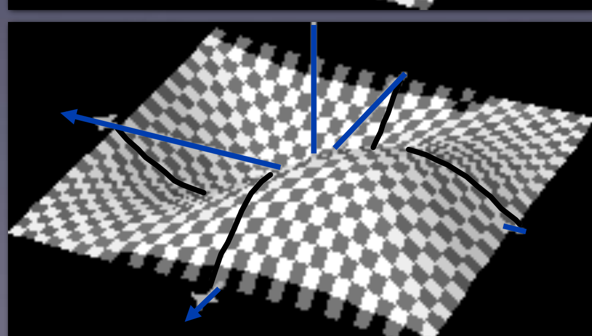
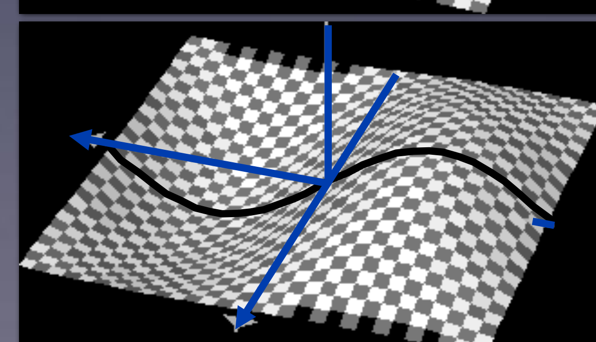
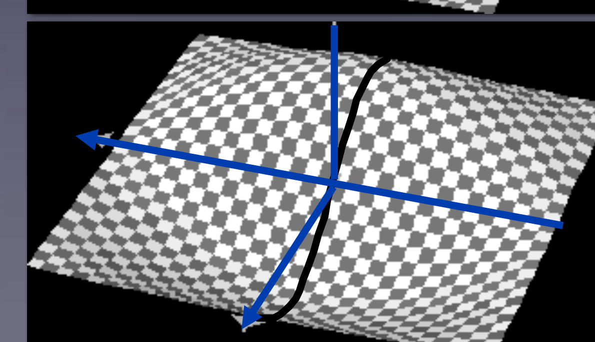


Degenerate waves





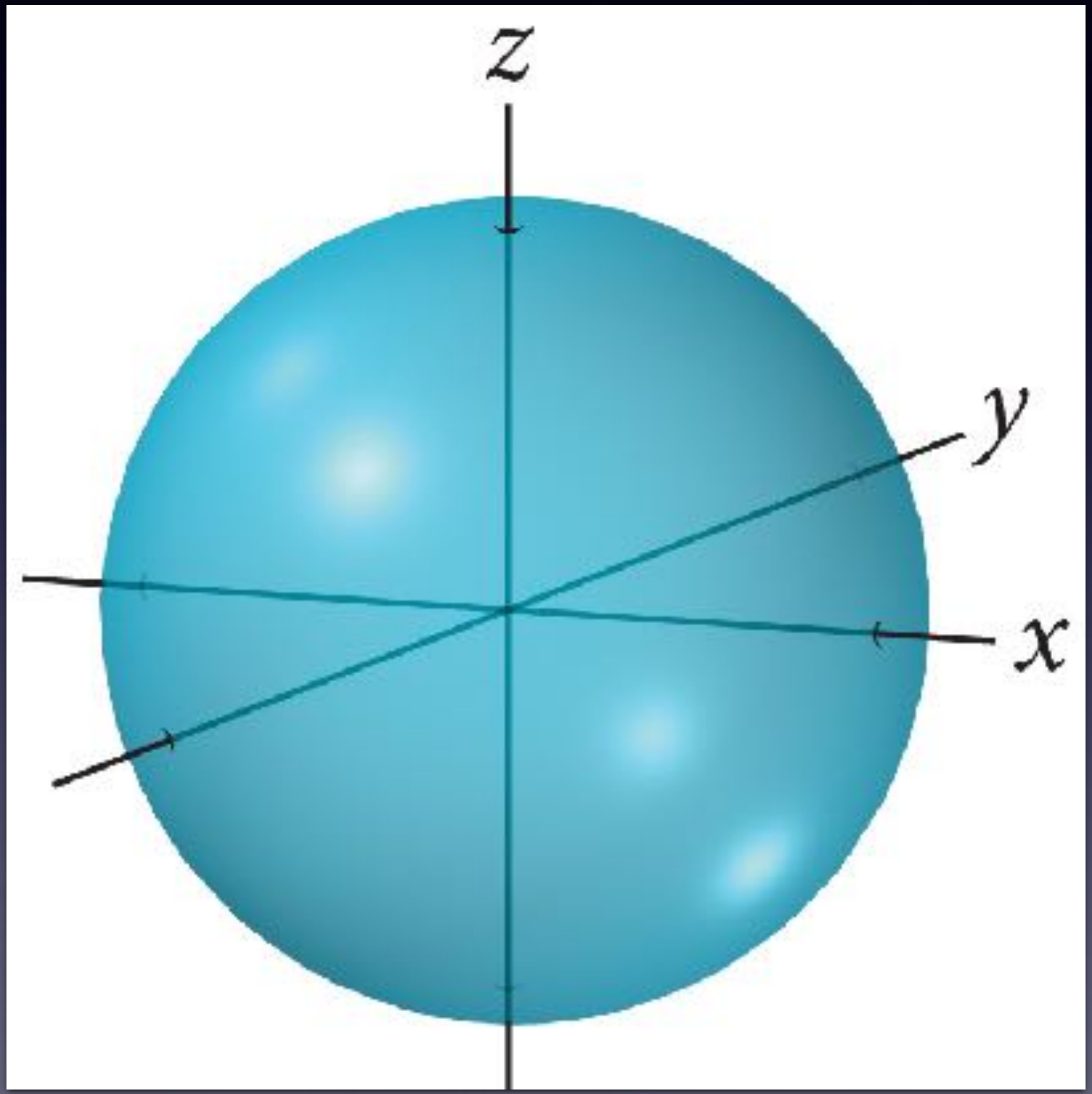
 =  + 

 =  − 

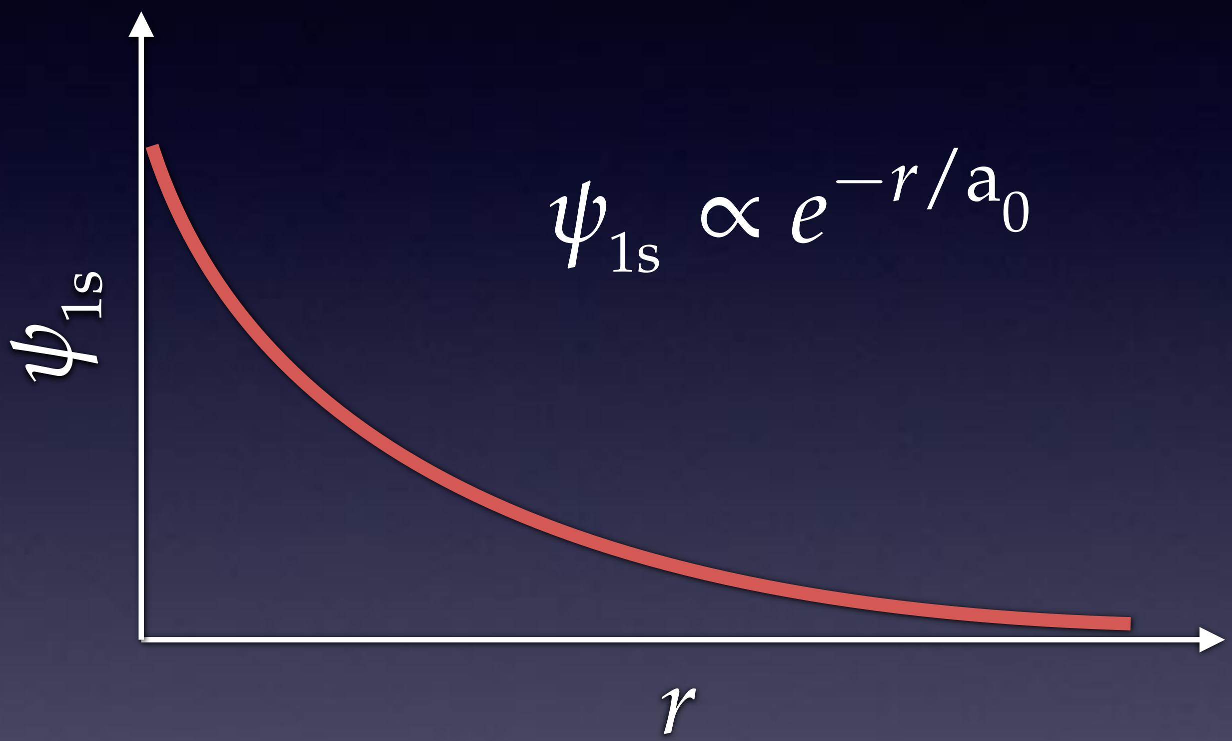
Review before we get to 3D

- Allowed waves are limited by the physical boundary conditions: Tie down ends, Stay inside box, etc.
- Higher Number of Nodes means Higher Energy
- In 2-D (and 3-D), Degenerate Sets are found for waves with angular nodes

Standing waves in three dimensions



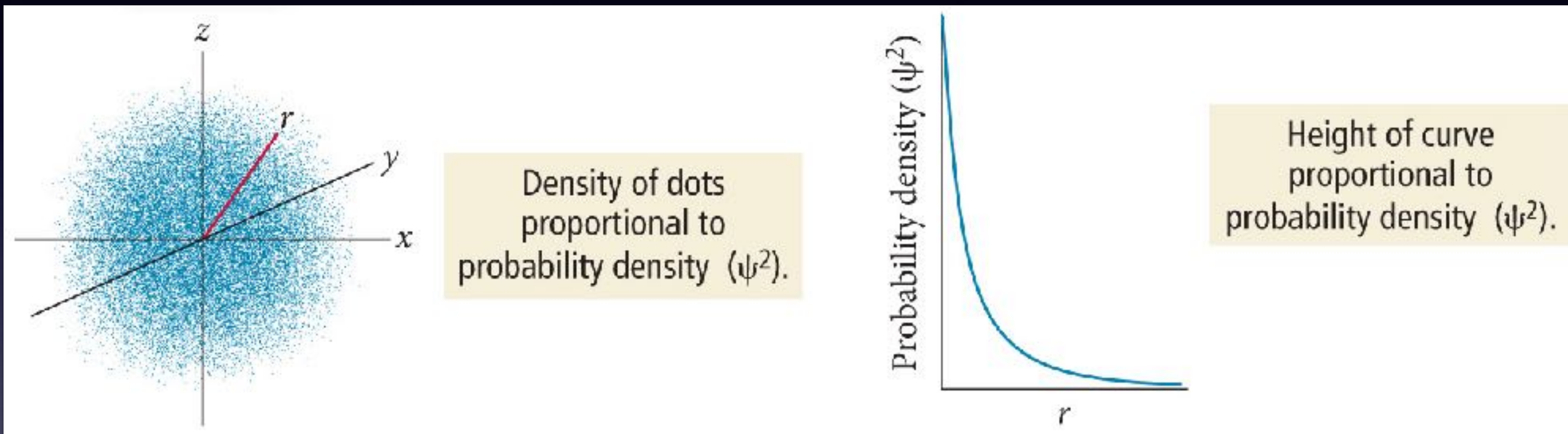
Tro, Fig. 7.24



Boundary condition is

$$\psi_{1s}(r = \infty) = 0$$

How do we “find” the electron?

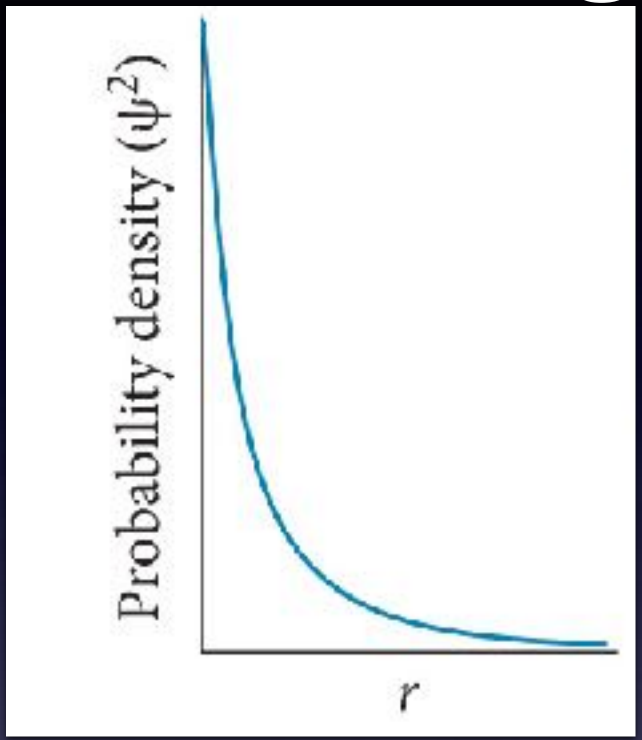


Tro, Fig. 7.23

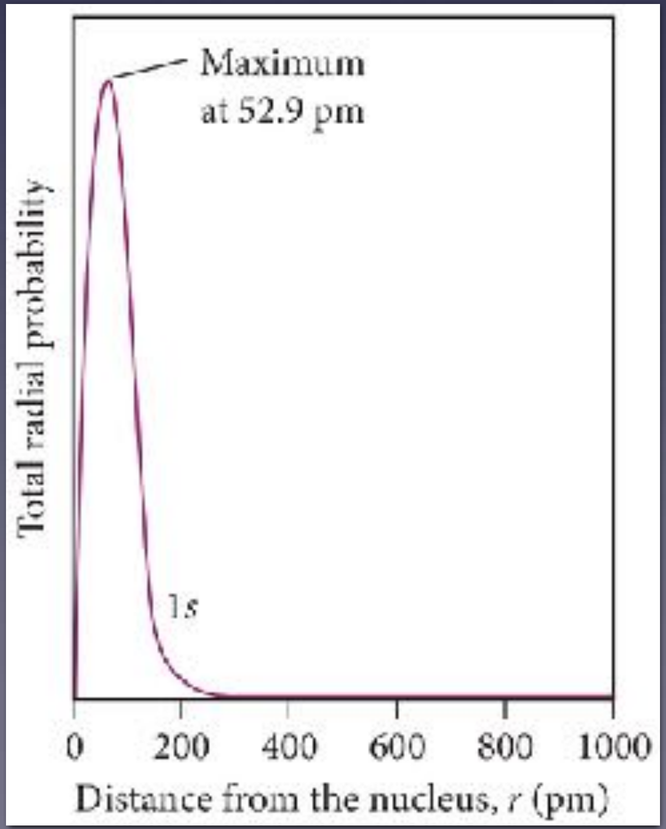
Wavefunction is $\psi_{1s} \propto e^{-r/a_0}$

But the likelihood of “finding” the electron in a particular region is given by ψ_{1s}^2.

Using ψ to localize electrons



Tro, Fig. 7.24 and 7.25



- Probability of finding an e⁻ in an area dτ:

$$\int \psi_{1s}^2 \, d\tau$$

- In spherical coordinates, that's:

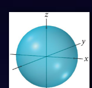
$$\int_r \int_\theta \int_\phi \psi_{1s}^2 \, r^2 \sin\theta \, dr \, d\theta \, d\phi$$

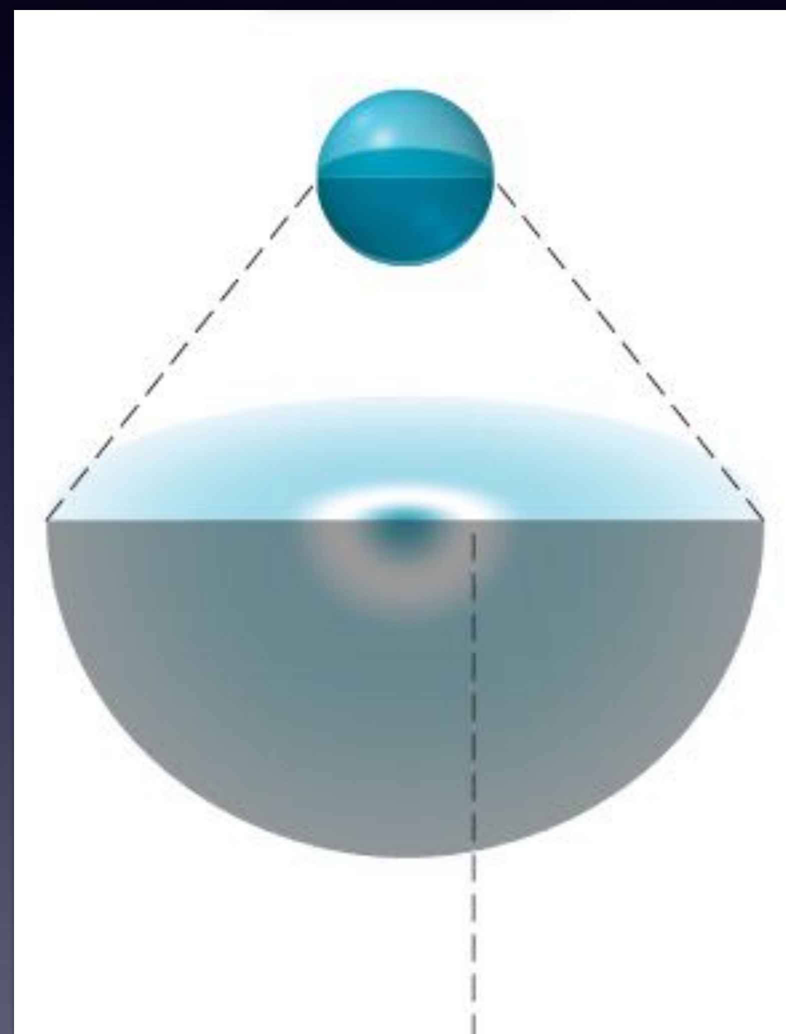
- If you only have radial parts (s-orbitals):

$$\int R_{1s}^2 r^2 \mathrm{d}r \quad \text{or} \quad \int 4\pi \psi_{1s}^2 r^2 \mathrm{d}r$$

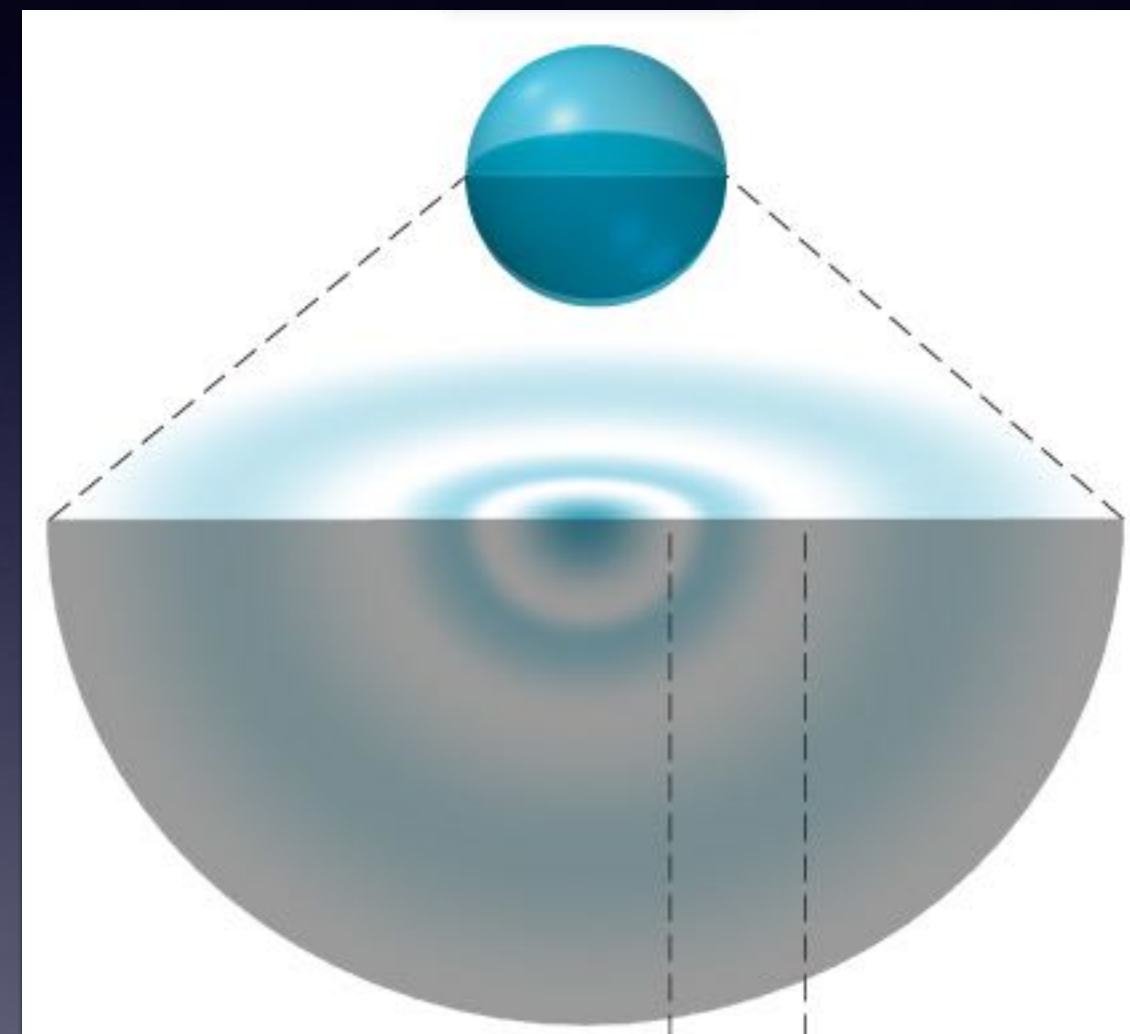
One kind of electron orbital

Tro, Fig. 7.24





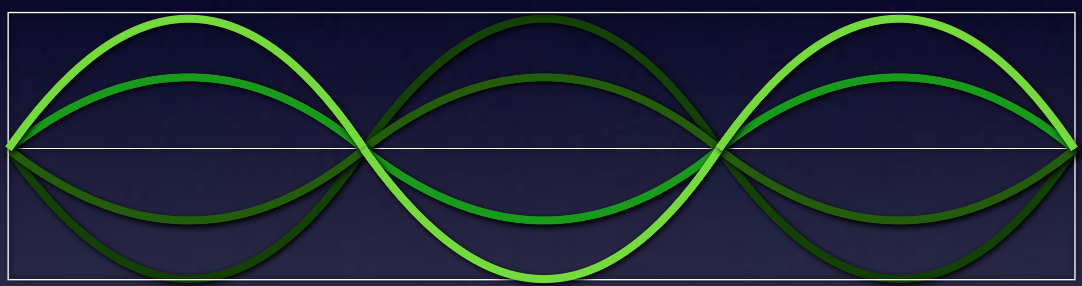
Tro, Fig. 7.26



How to we define the differences between them?

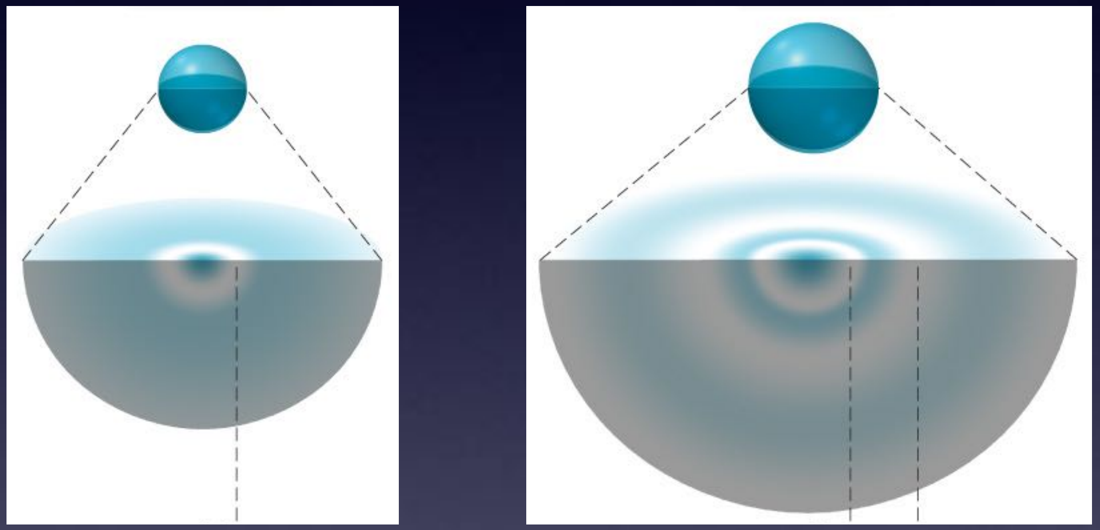
Principal quantum number, n

In one dimension:



$$\psi(x,t) = A\sin\left(\frac{n\pi x}{d}\right),\ n = 3$$

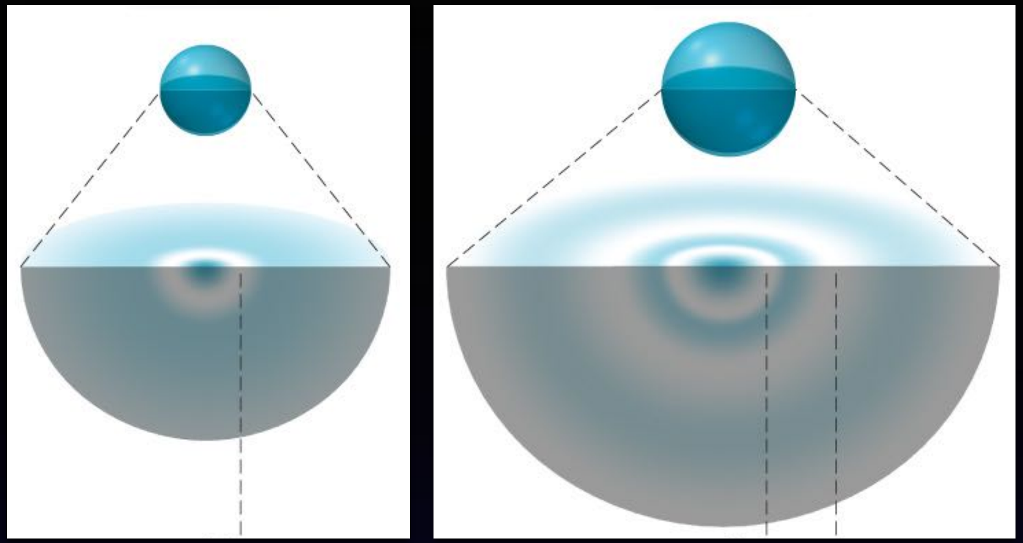
In three dimensions:



Tro

- Takes positive integer values n = 1, 2, 3, 4, .. , ∞
- Conveys information about orbital **size** and **energy**.

Fig. 7.26
Tro



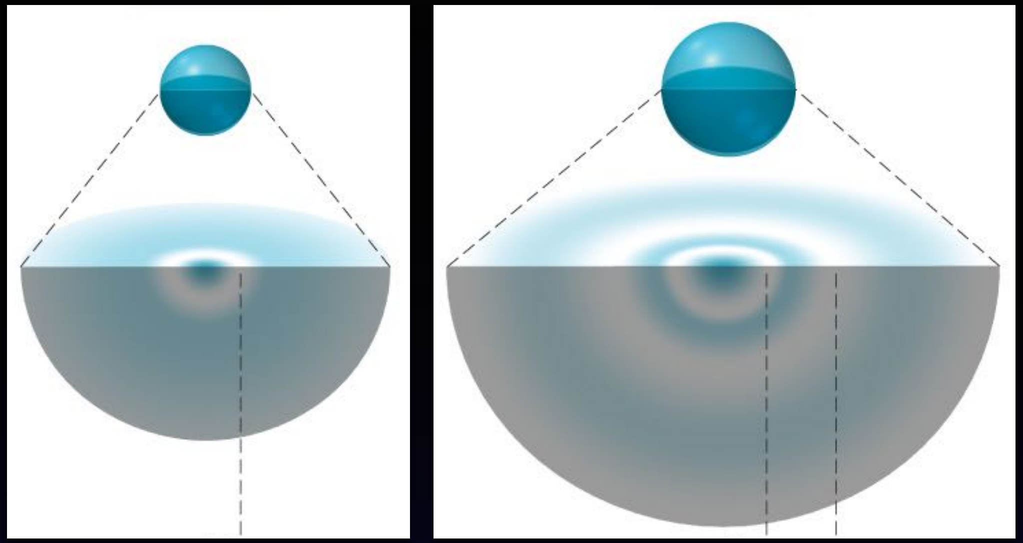
Now you try…

- What is the dimensionality of the nodes for 3-dimensional waves?

- For the orbitals above, what geometrical shape describes the nodes?

- How do the number of nodes relate to the principle quantum number, n?

Fig. 7.26
Tro



Now you try…

- What is the dimensionality of the nodes for 3-dimensional waves?

2-dimensional

- For the orbitals above, what geometrical shape describes the nodes?

Sphere (surface)

- How do the number of nodes relate to the principle quantum number, n?

total nodes = $n - 1$

Where did we go today?

Ch1010-A17-A03 Lecture 5

- Quantistry continued!
- § 2.6 Quantum numbers
- § 2.6 Atomic orbitals:
  Shapes, sizes, smells, etc.

Next time…

- § 3.3 Filling electrons in orbitals

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Mathematica images credit

Nathan S. Lewis
Professor, Caltech

Image from nsl.caltech.edu