THE HYDROGEN ATOM

General Chemistry I, Lecture Series 5

Qixi Mi

Reading:
OGB8 §5.1

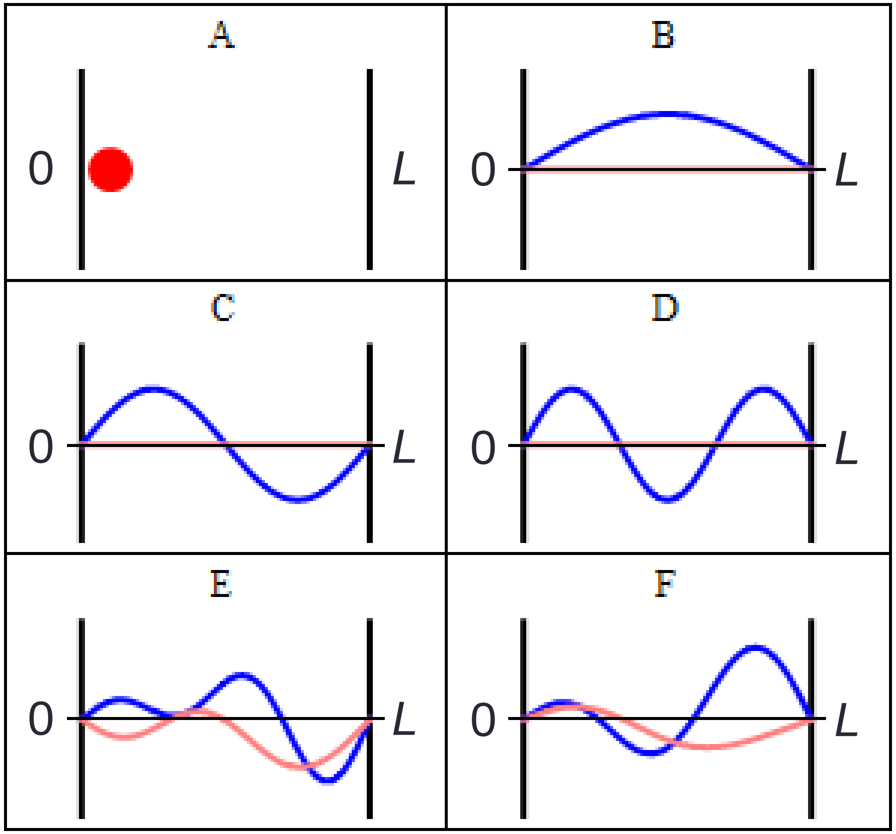
Outline

- Oscillations in 2D
- Atomic orbitals: Appearance
- Atomic orbitals: Properties

1D Standing Wave (1)

(1) $\psi(x) = 0$ for $x \le 0$ or $x \ge L$ (Boundary condition 边界条件)

(2) $\int |\psi(x)|^2 \, dx = 1$

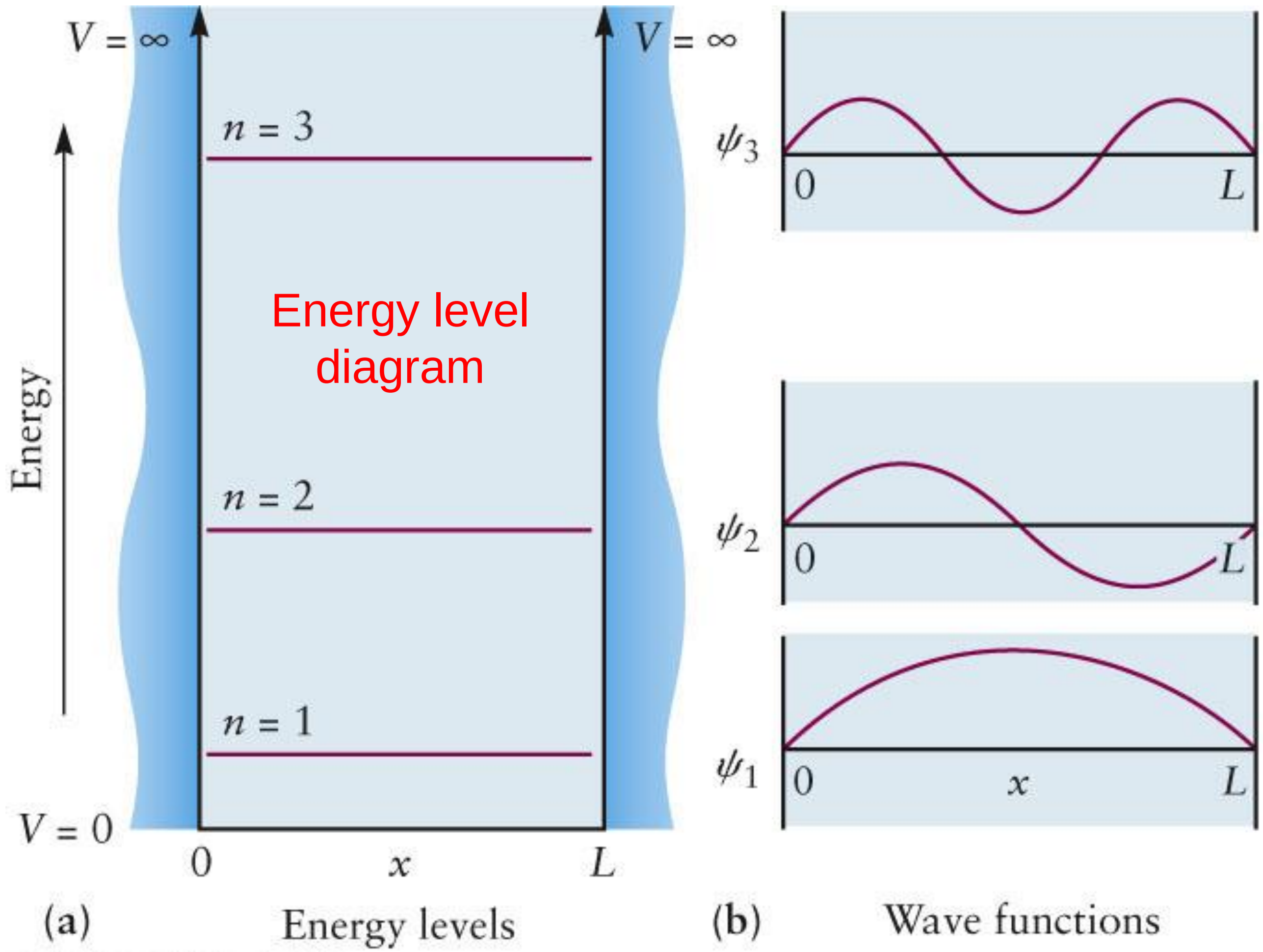


Stationary states 定态

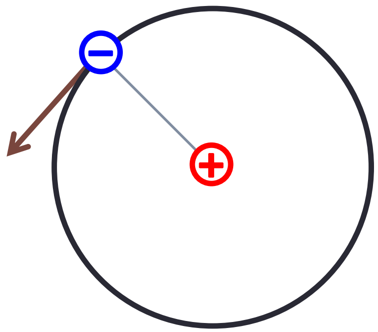
Time-dependent state

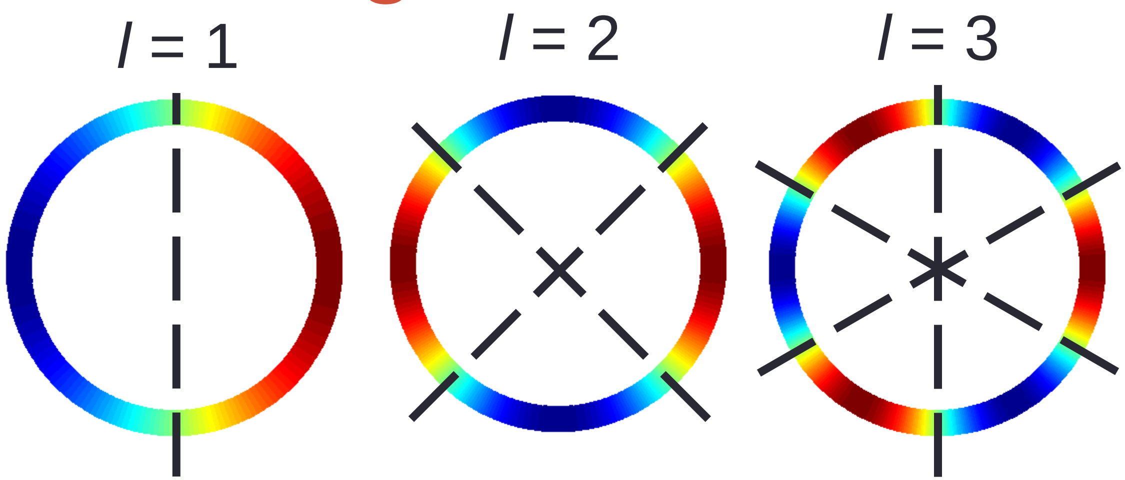
1D Standing Wave (2)

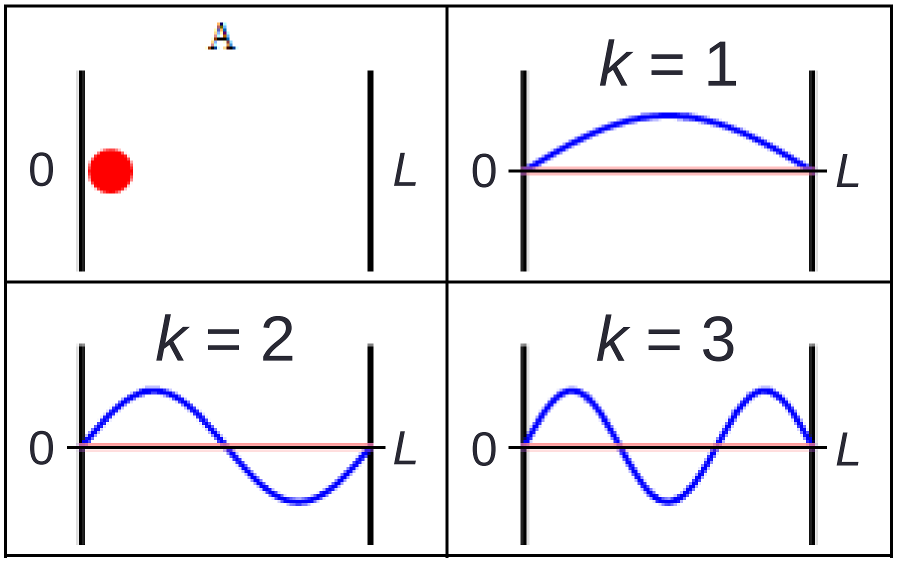
The n^{th} Wave function: $\psi_n(x) \propto \sin\left(n\pi \frac{x}{L}\right)$, n = number of nodes + 1.

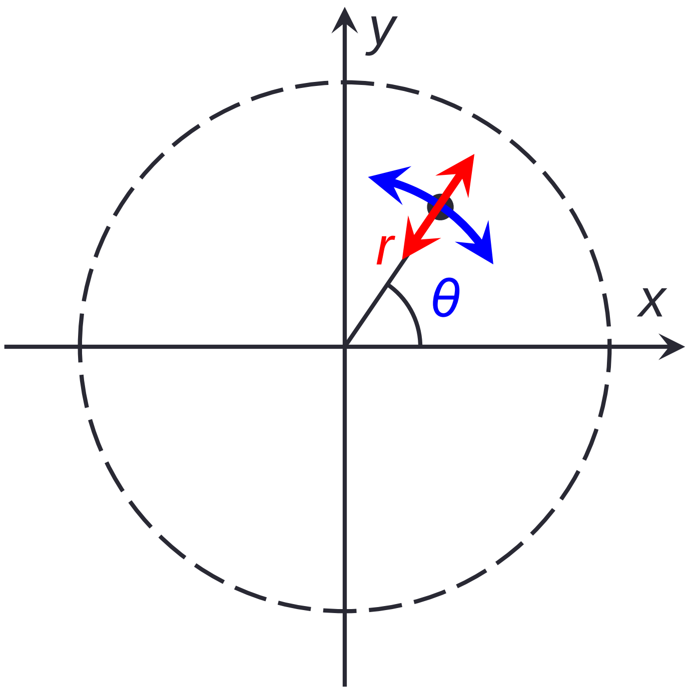


From 1D to 2D Standing Waves







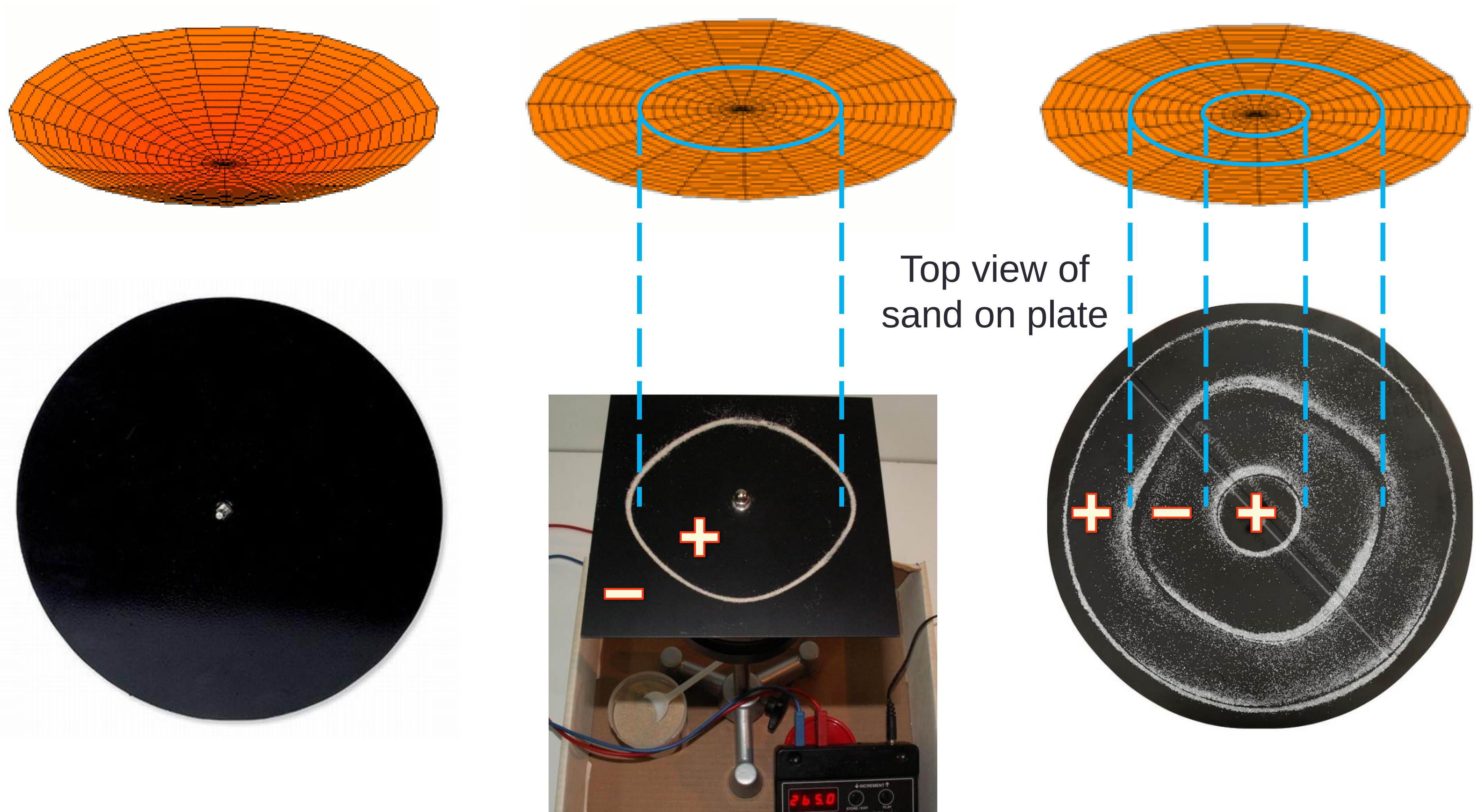


Oscillations of a Round Plate

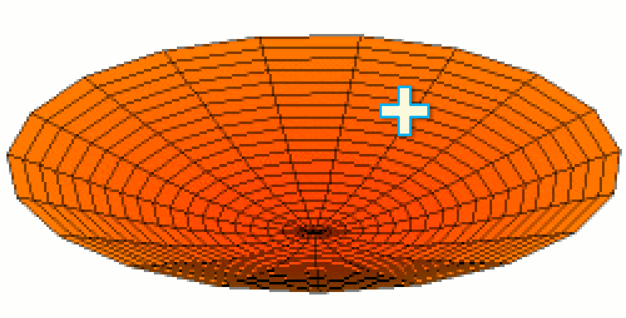
No nodes

1 nodal ring
(radial node)

2 nodal rings



The 1s Wave



主量子数
Principal quantum number n =
Total number of nodes + 1

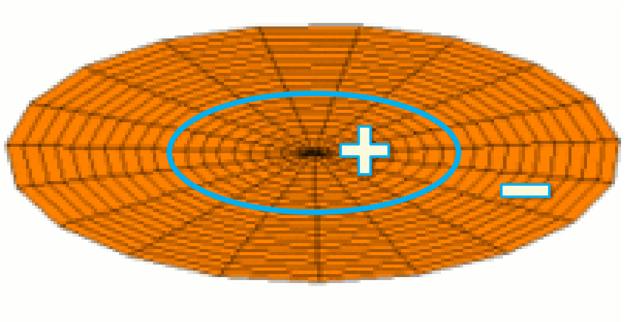
角(动量)量子数
Angular quantum number l =
Number of angular nodes

$l = 0, 1, 2, 3\ldots \Rightarrow s, p, d, f\ldots$

No nodes.

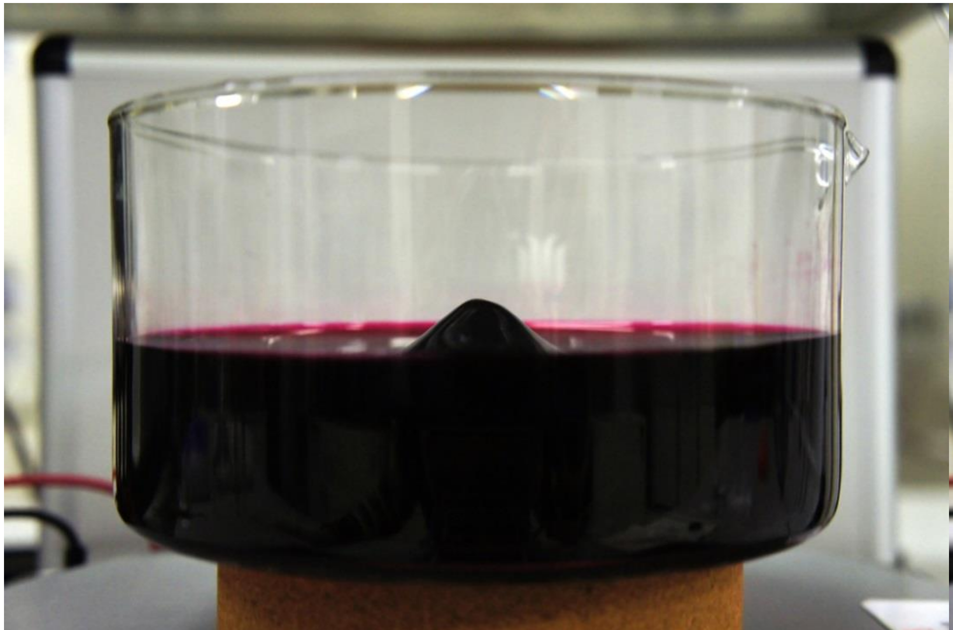
$n = 1, l = 0 \Rightarrow 1s$

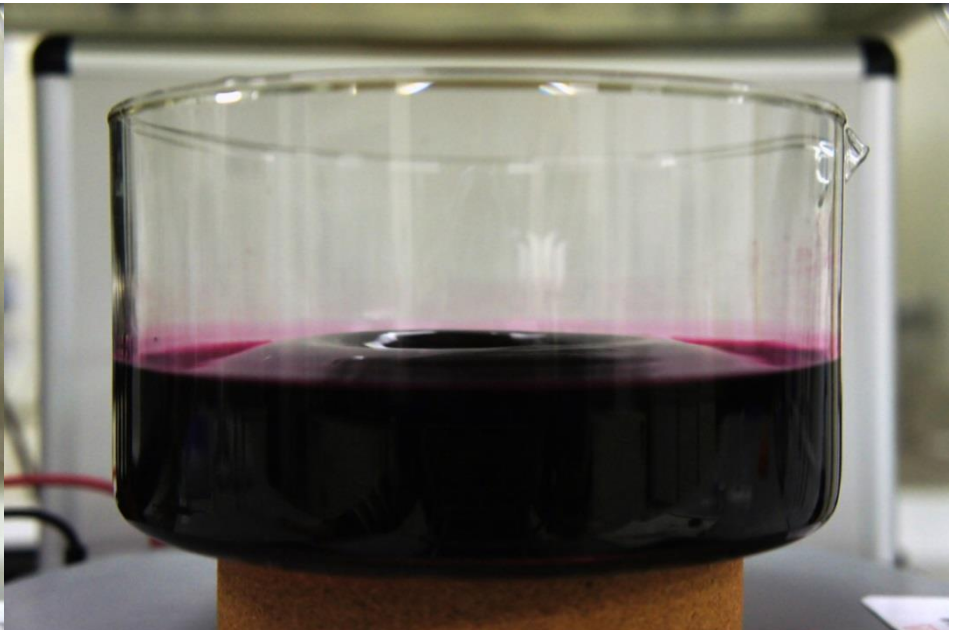
The 2*s* Wave



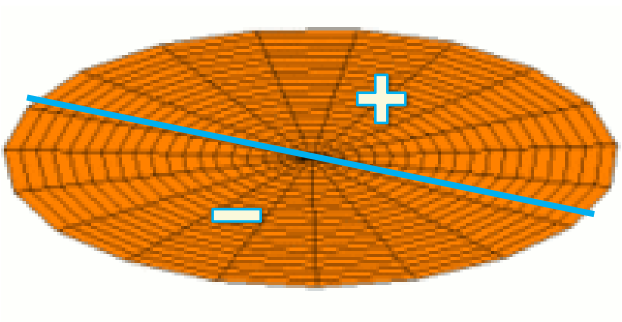
1 nodal ring (radial node)

$n = 2, l = 0 \Longrightarrow 2s$



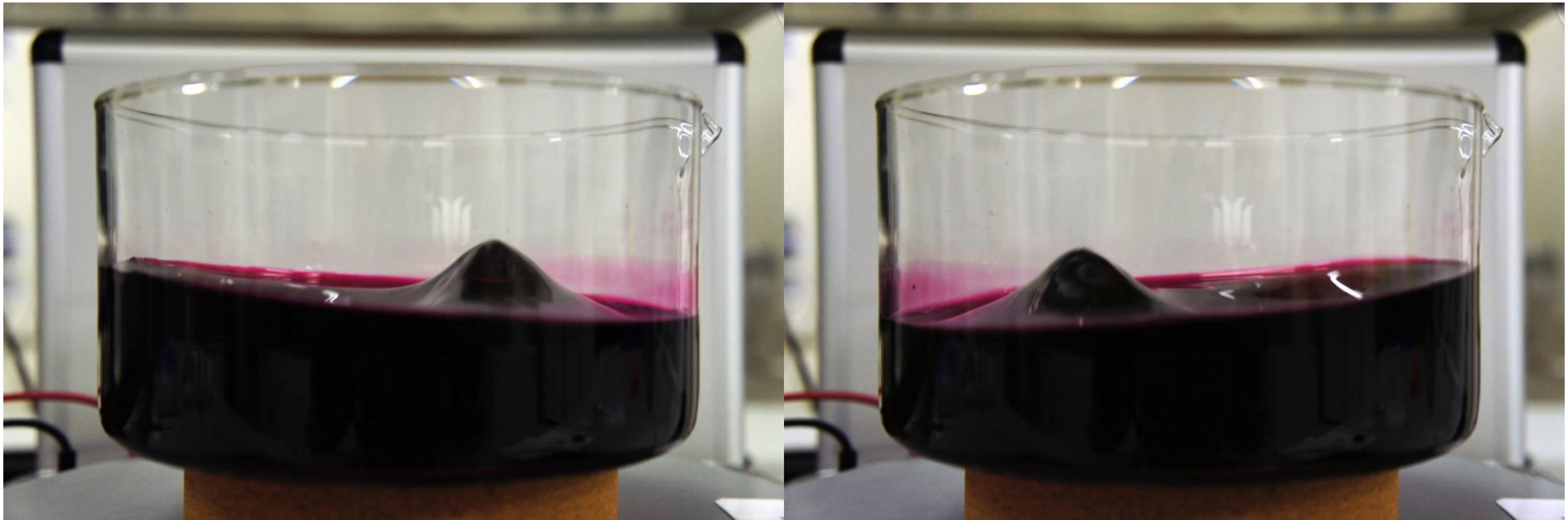


The 2*p* Wave

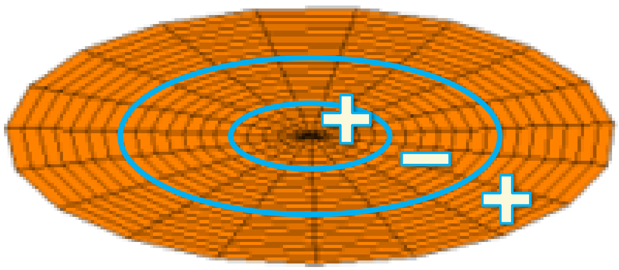


1 nodal line (angular node)

$n = 2, l = 1 \implies 2p$

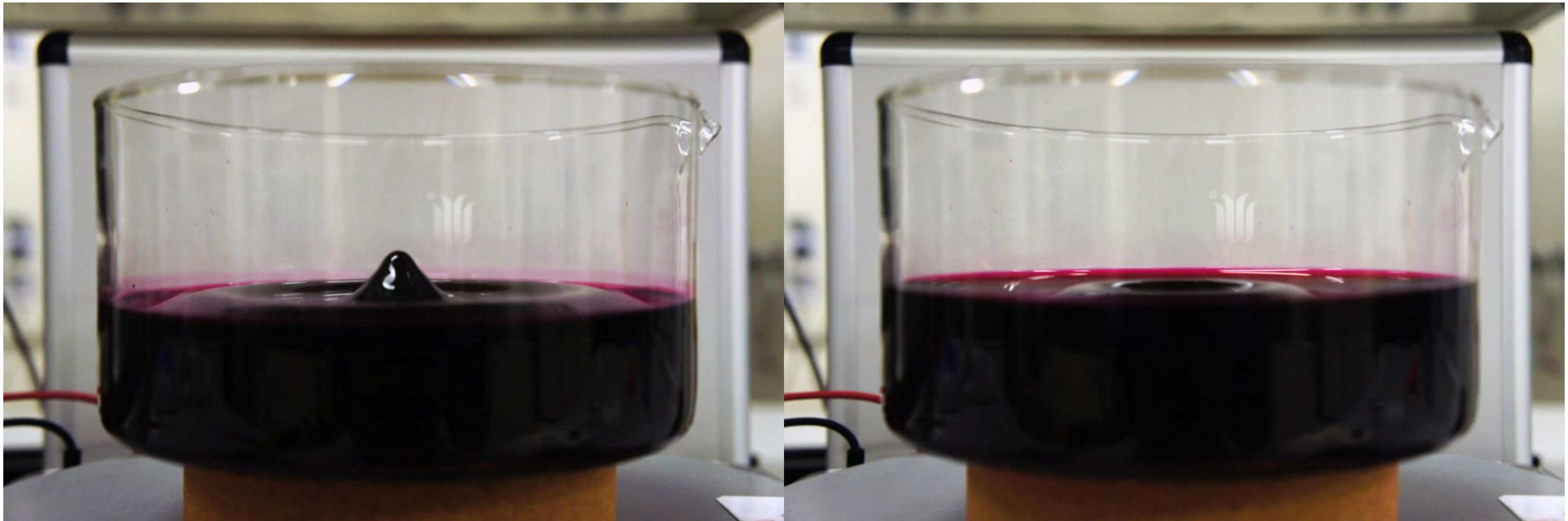


The 3s Wave

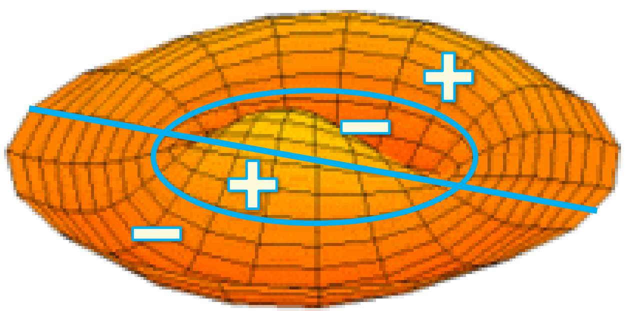


2 nodal rings (radial nodes)

$n = 3, l = 0 \implies 3s$



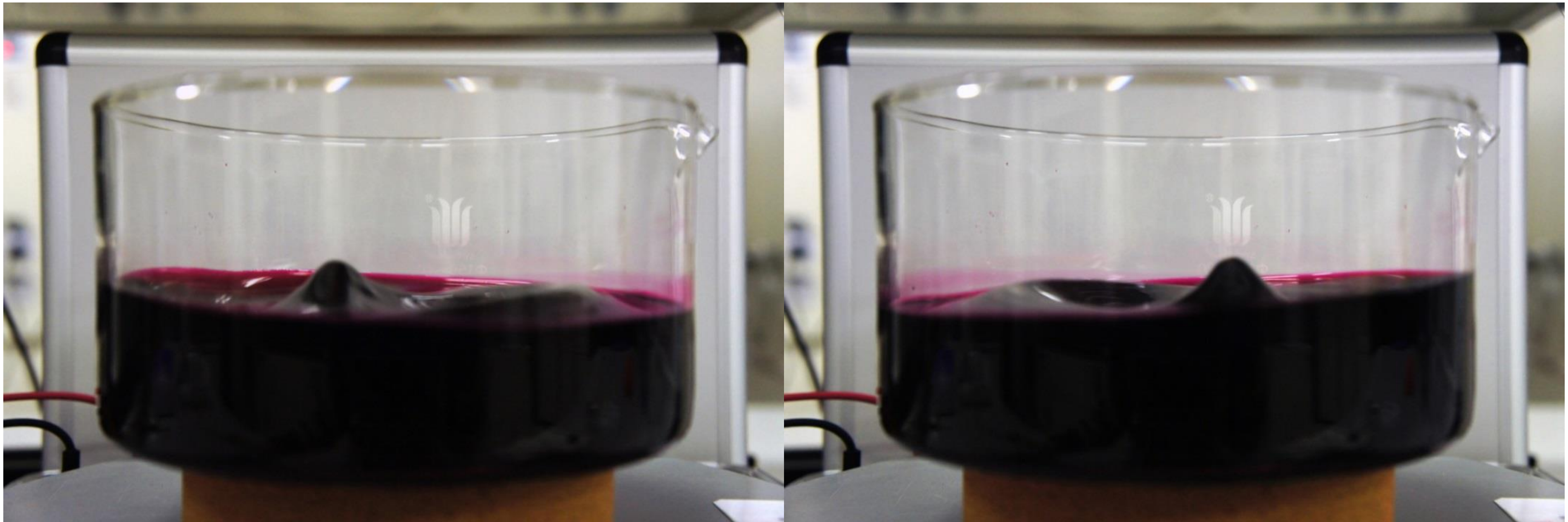
The 3*p* Wave



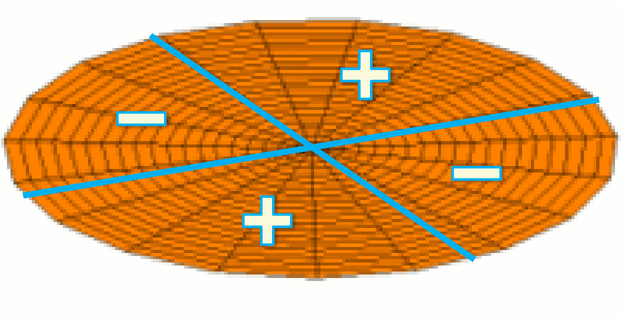
1 nodal ring (radial node)

1 nodal line (angular node)

$n = 3, l = 1 \implies 3p$

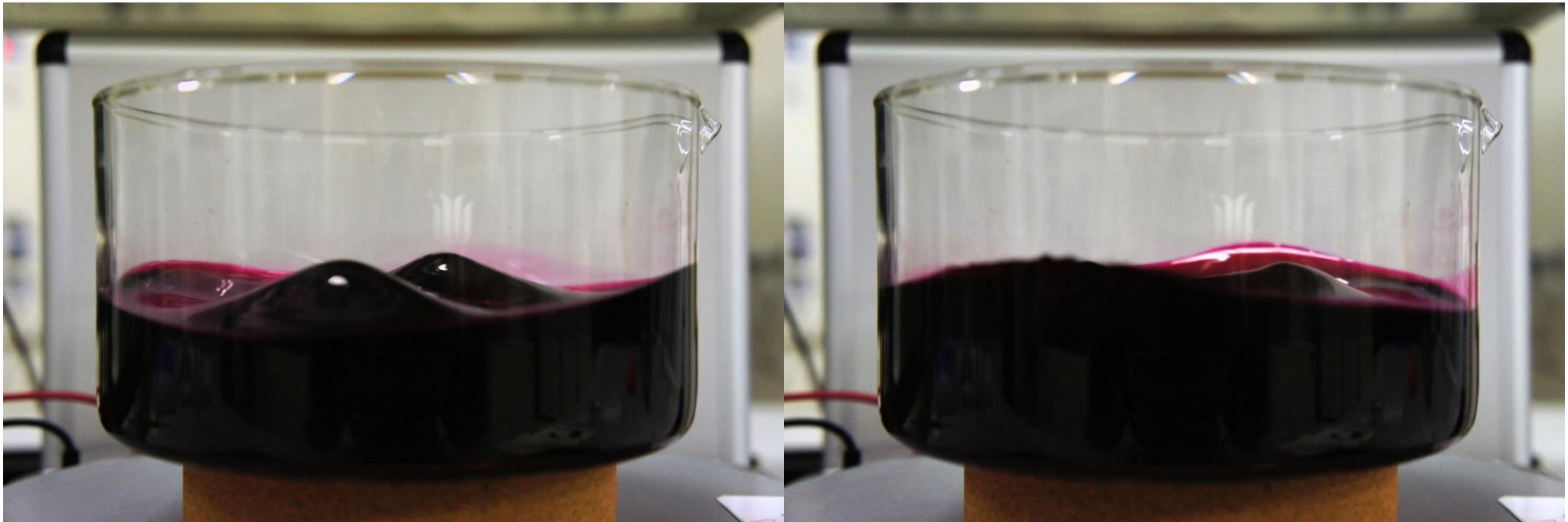


The 3*d* Wave



2 nodal lines (angular nodes)

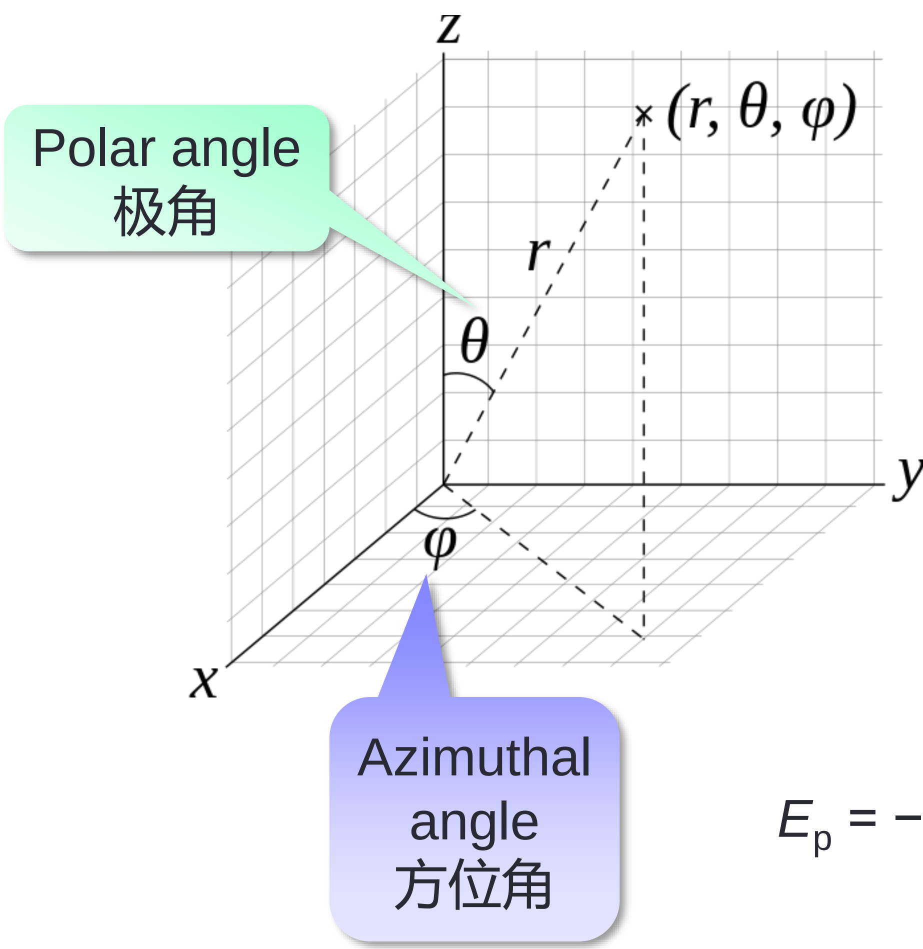
$n = 3, l = 2 \implies 3d$

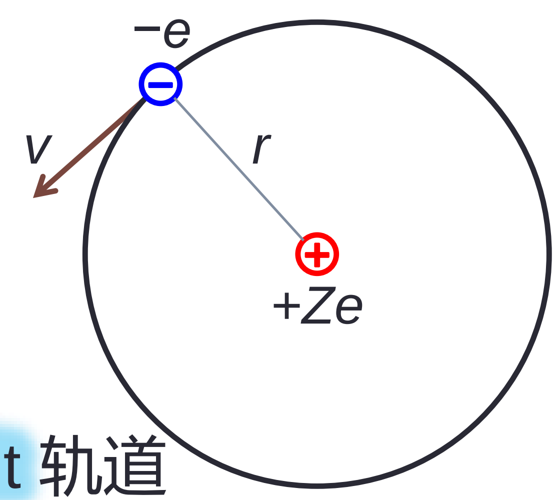


Outline

- Oscillations in 2D
- Atomic orbitals: Appearance
- Atomic orbitals: Properties

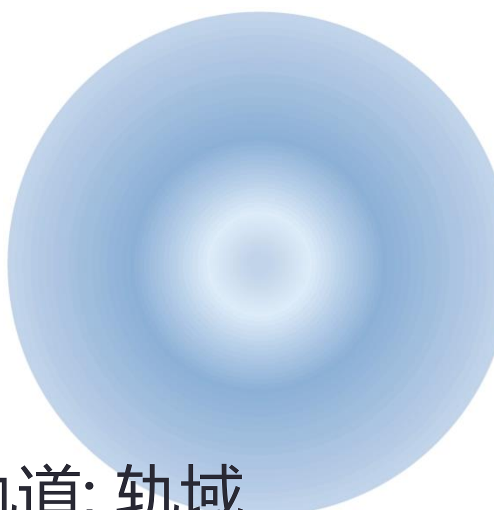
Spherical Polar Coordinates 球极坐标





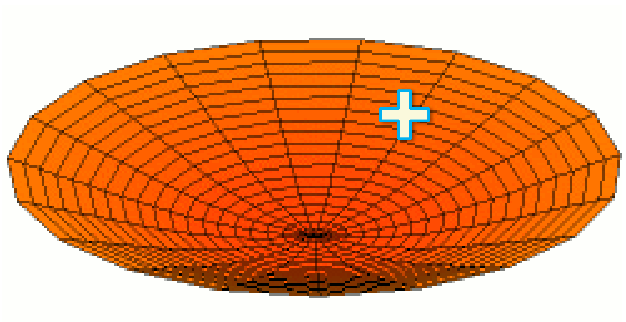
Orbit 轨道

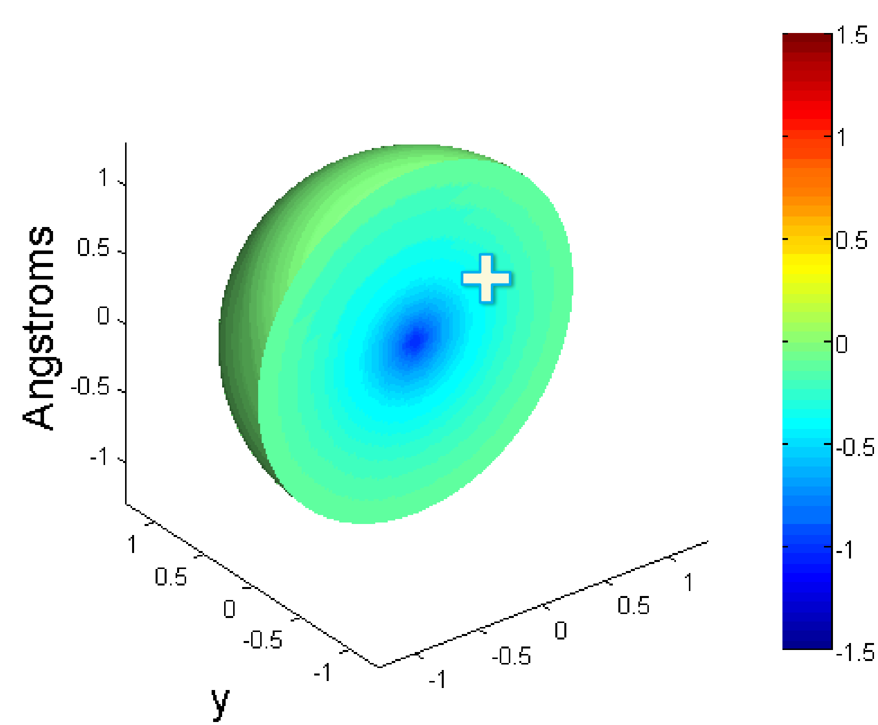
$$E_p = -\frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r}$$



Orbital 轨道; 轨域

The 1s Wave in 3D

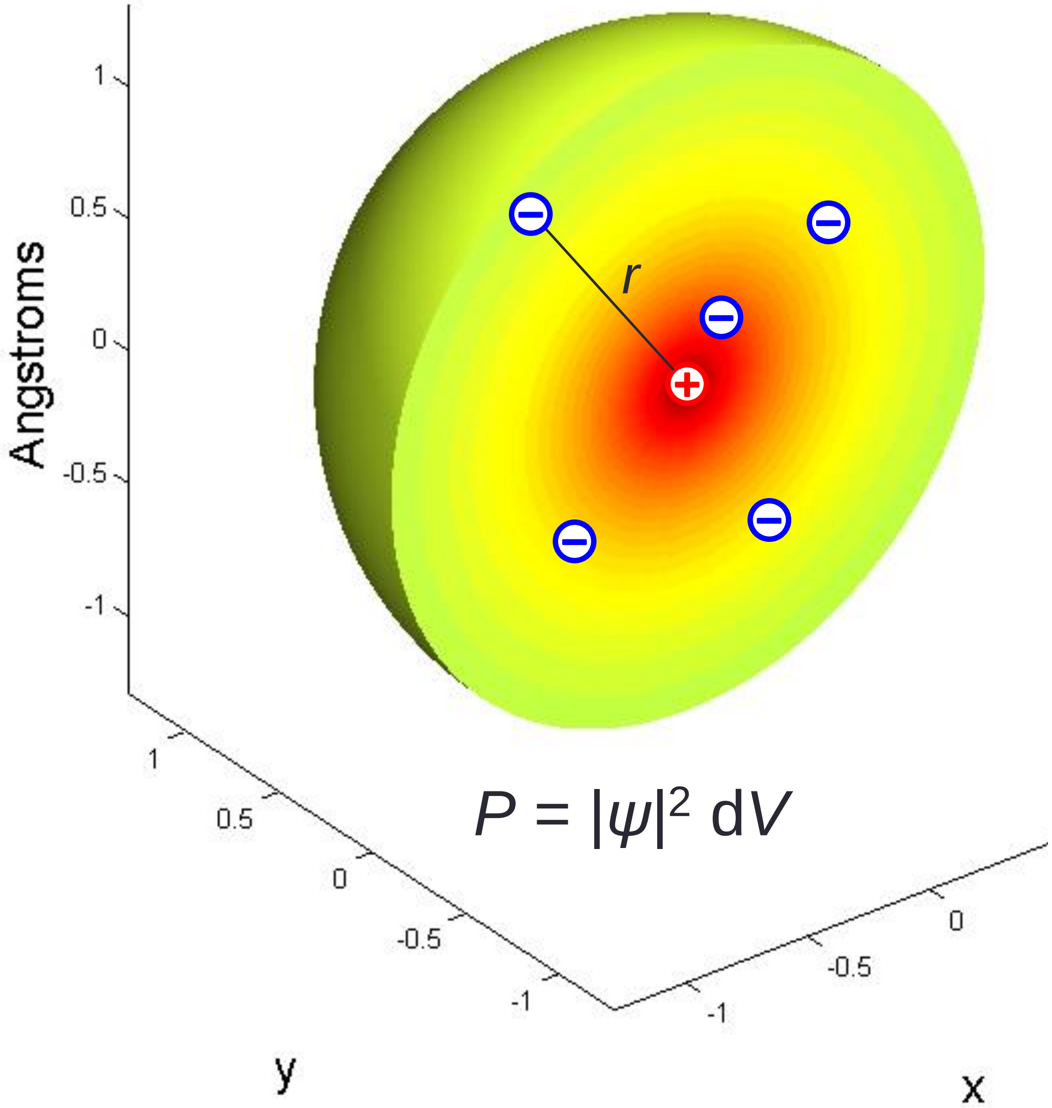




No nodes.

$n = 1, l = 0 \Longrightarrow 1s$

Wave Function of the 1s Orbital

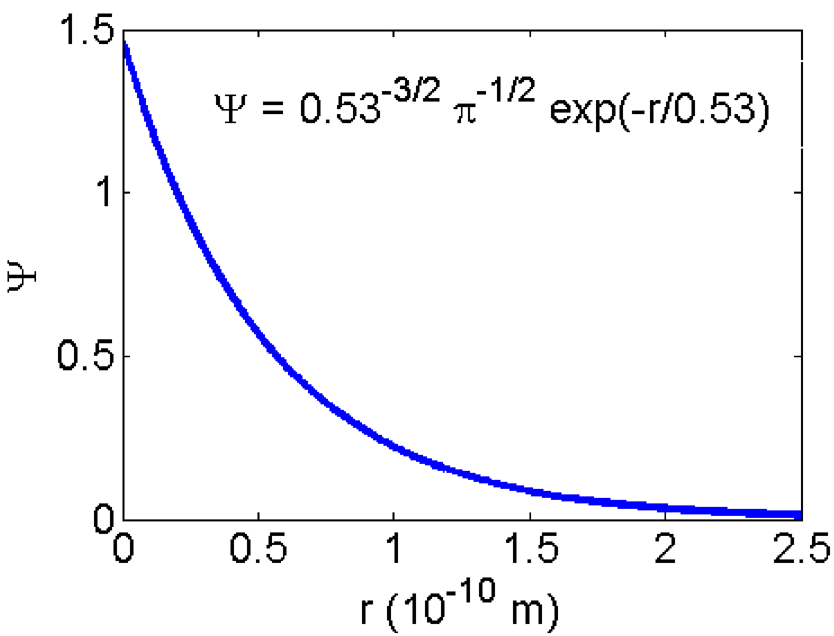


$P = |\psi|^2 \, dV$

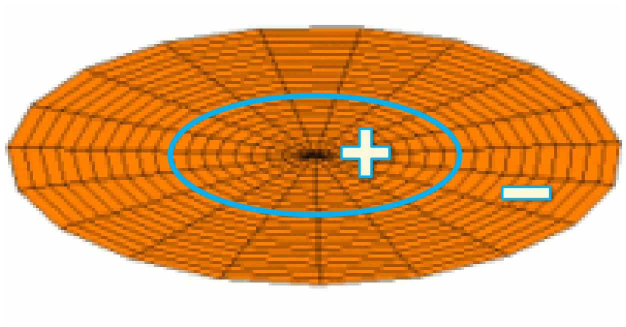
$$\psi_{1s} = \frac{1}{\sqrt{\pi}} a_0^{-3/2} \cdot \exp\left(-\frac{r}{a_0}\right)$$

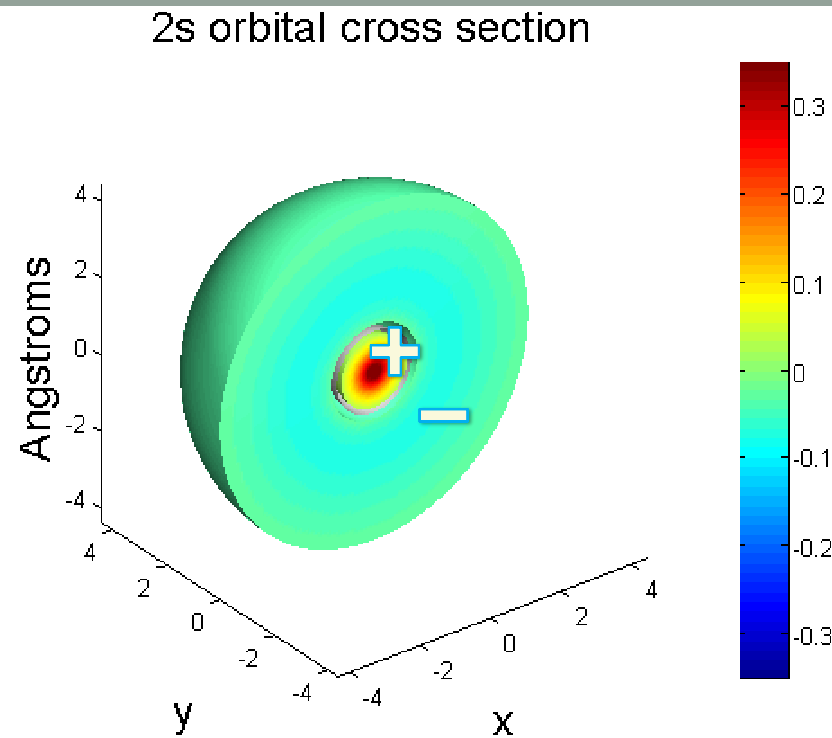
Bohr radius a_0 = 53 pm = 0.53 Å

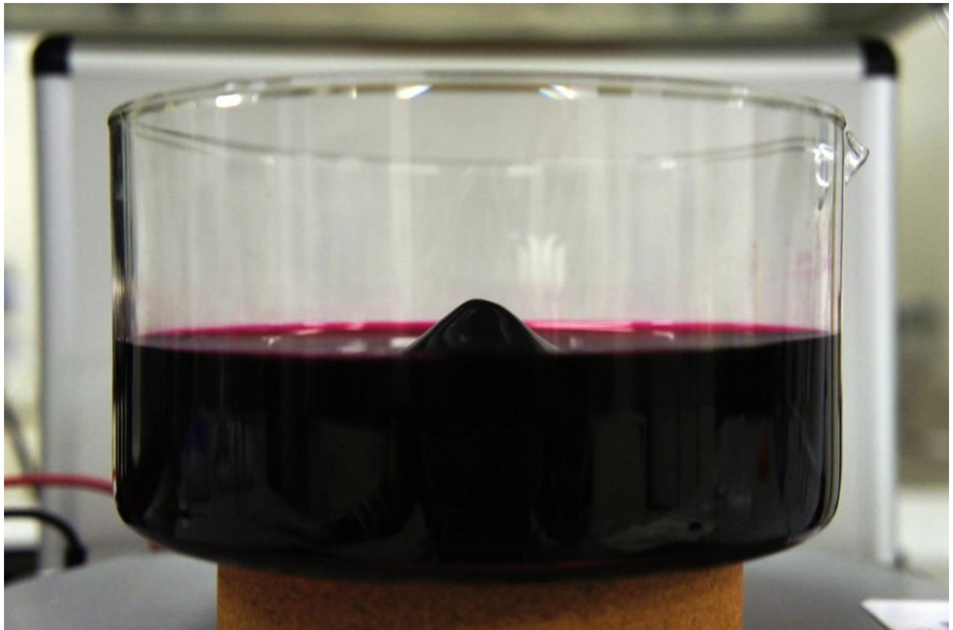
1 Ångstrom = 10^{-10} m



The 2*s* Wave in 3D



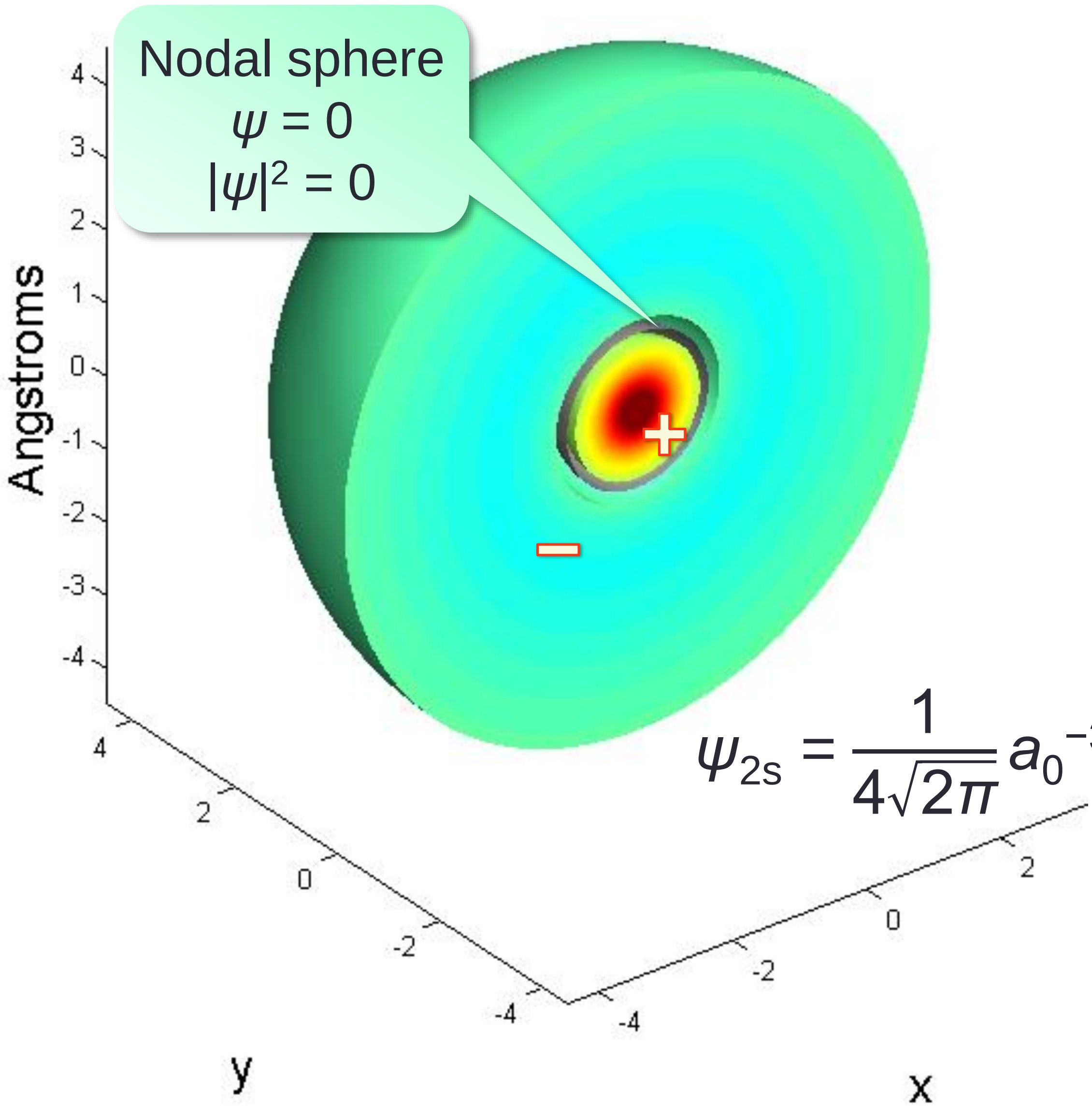


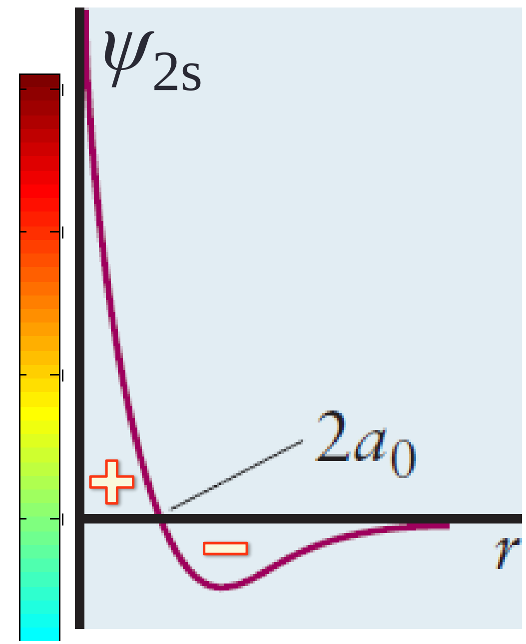


1 nodal sphere (radial node)

$n = 2, l = 0 \Longrightarrow 2s$

Wave Function of the 2*s* Orbital





$$\psi_{2s} = \frac{1}{4\sqrt{2\pi}} a_0^{-3/2} \cdot \left(2 - \frac{r}{a_0}\right) \exp\left(-\frac{r}{2a_0}\right)$$

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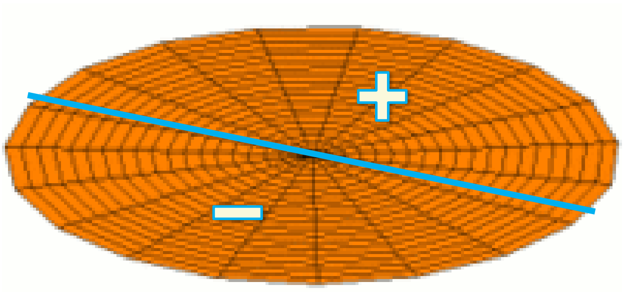
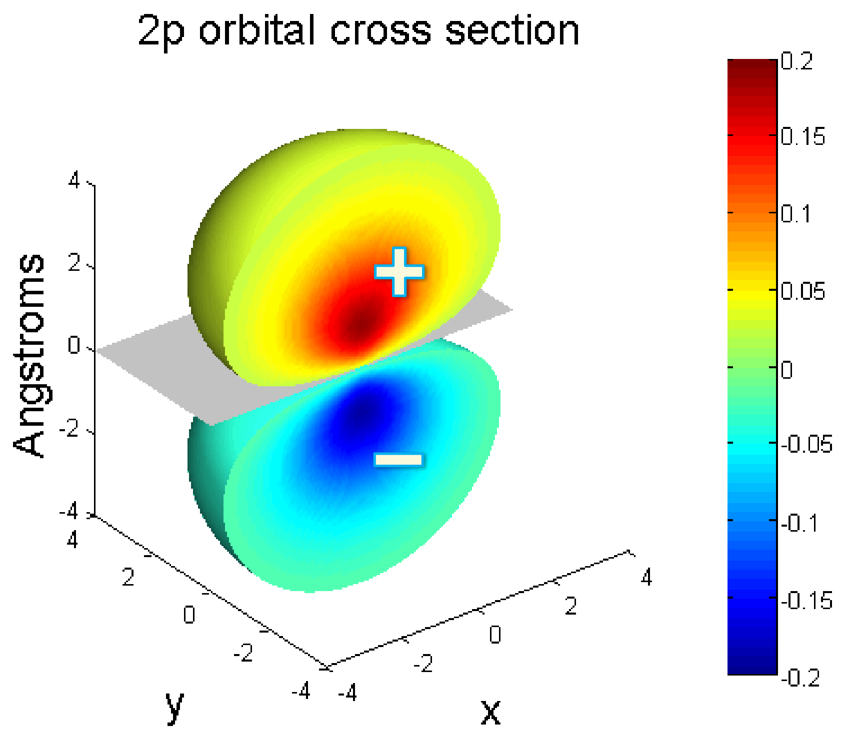
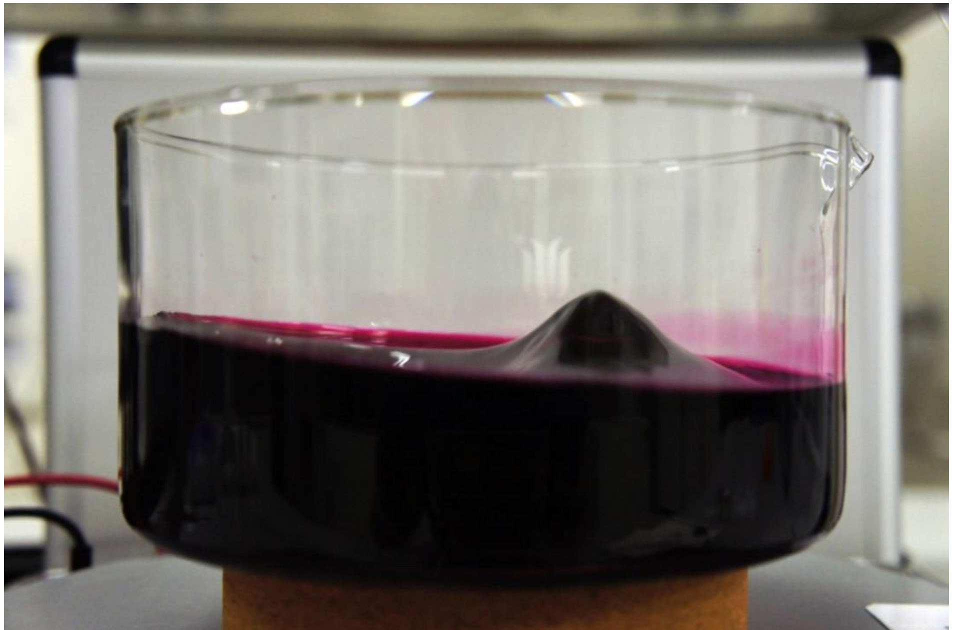
The 2*p* Wave in 3D





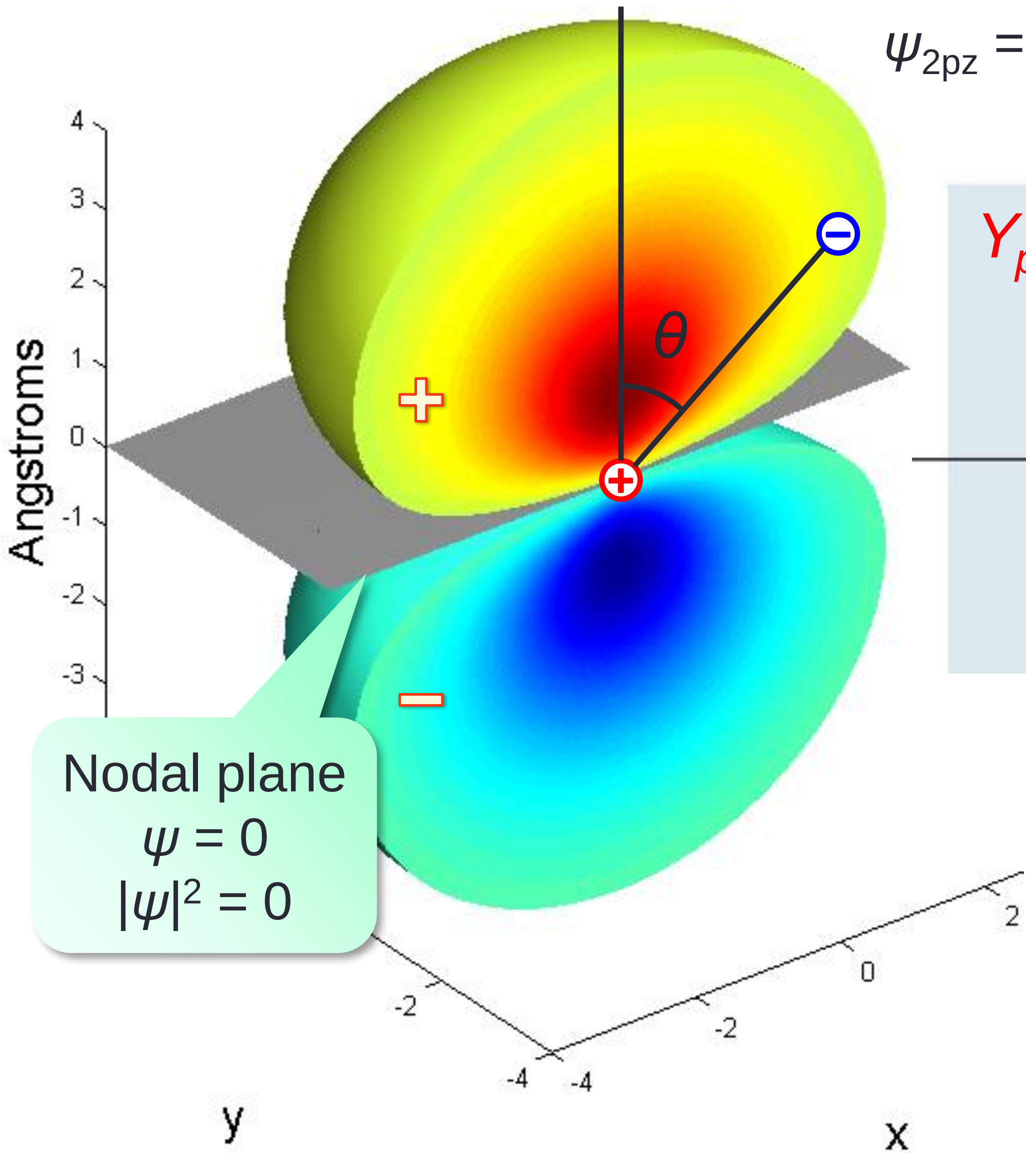


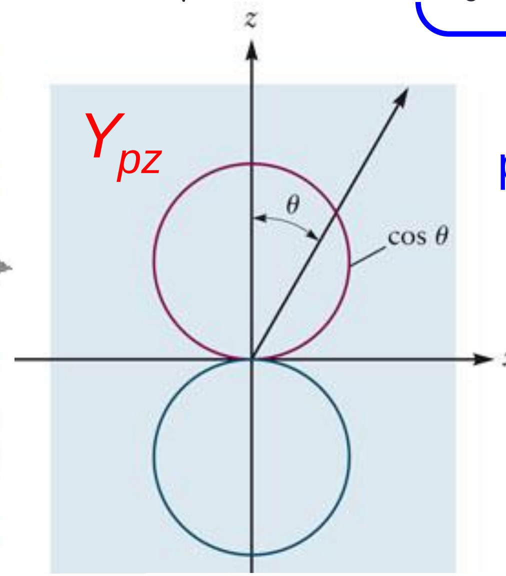
1 nodal plane (angular node)

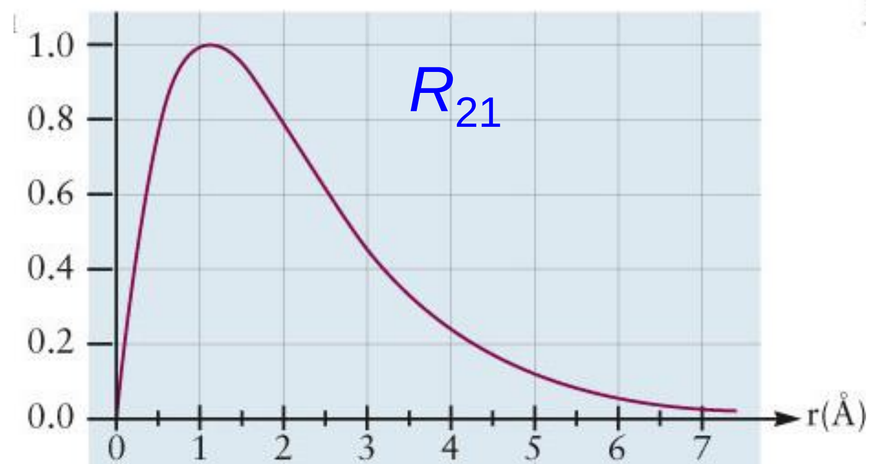
$n = 2, l = 1 \implies 2p$

Wave Function of the 2p_z Orbital

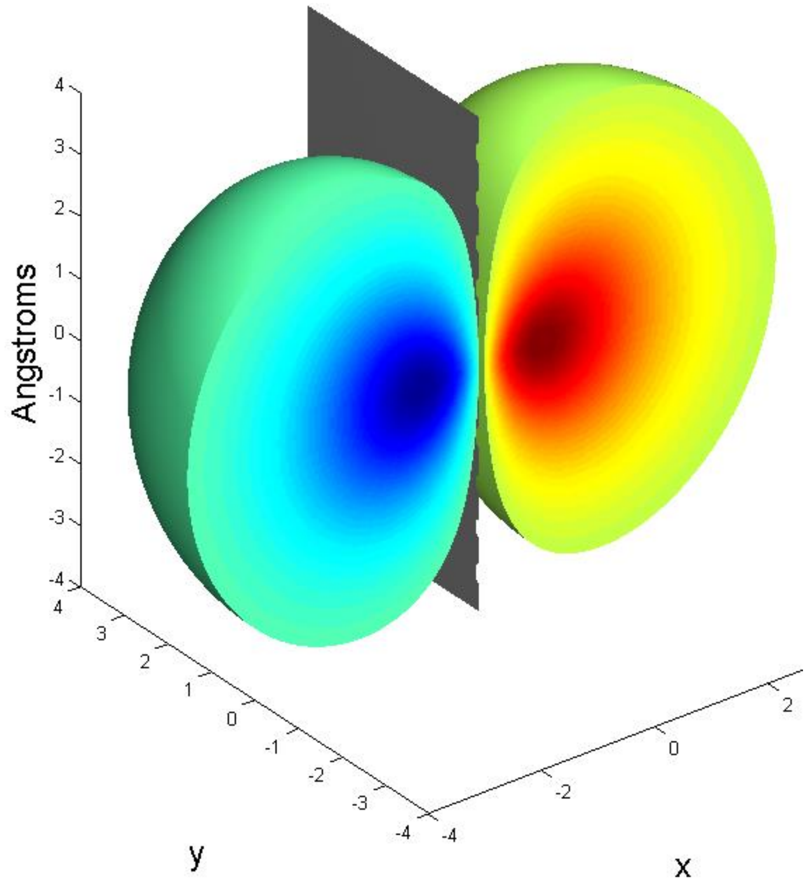
$$\psi_{2pz} = \frac{1}{4\sqrt{2\pi}} a_0^{-3/2} \cdot \underbrace{\frac{r}{a_0} \exp\left(-\frac{r}{2a_0}\right)}_{\text{Radial part, } R_{21}} \cdot \underbrace{\cos\theta}_{\text{Augular part, } Y_{pz}}$$



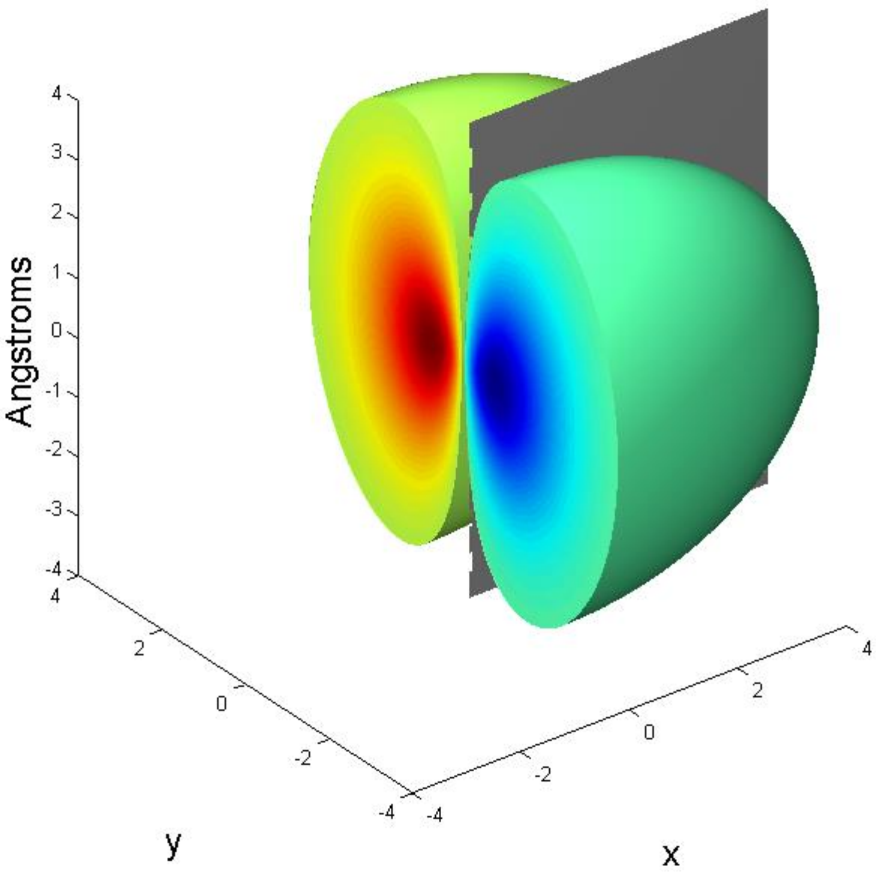




The 2p_x and 2p_y Orbitals

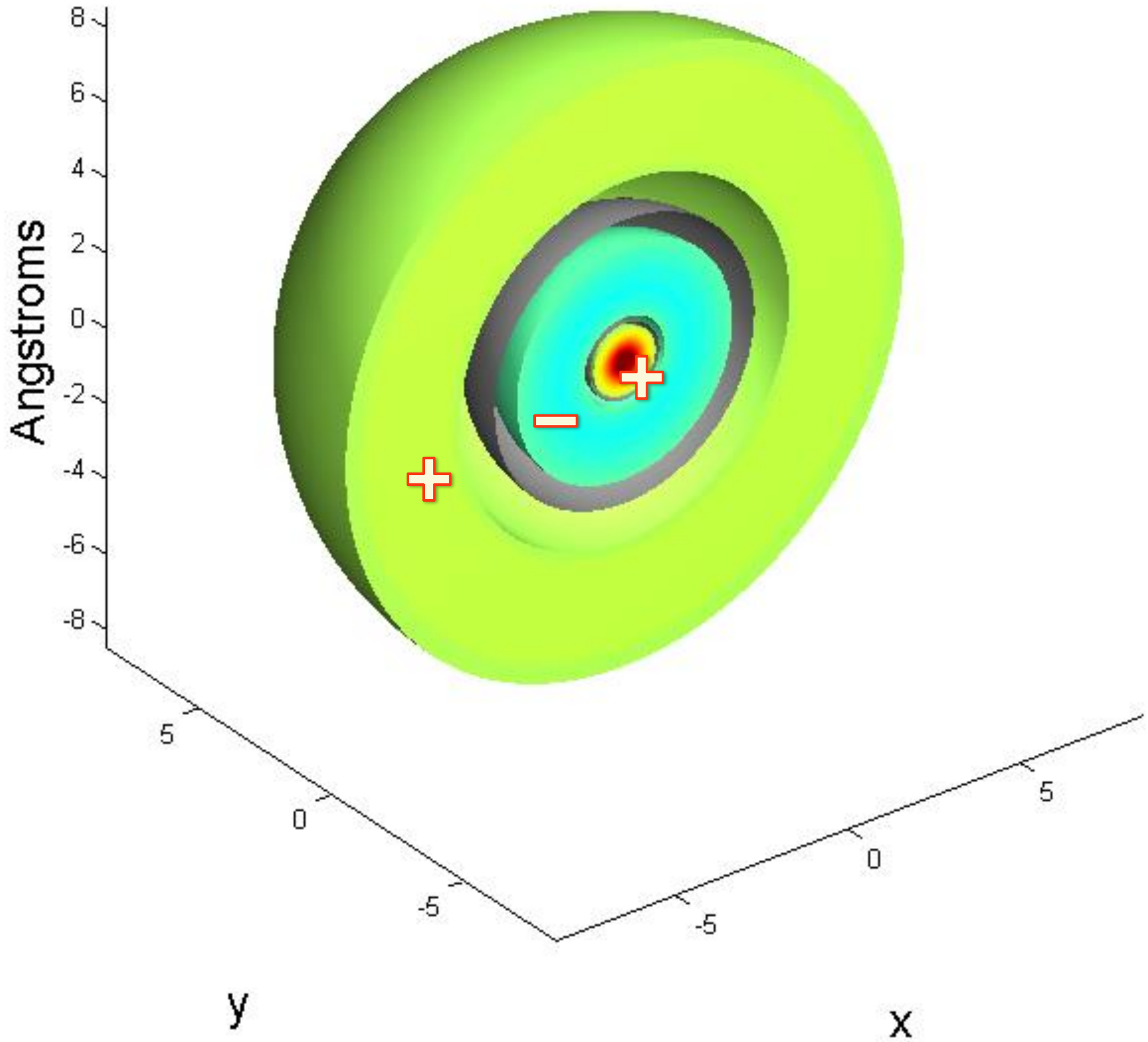


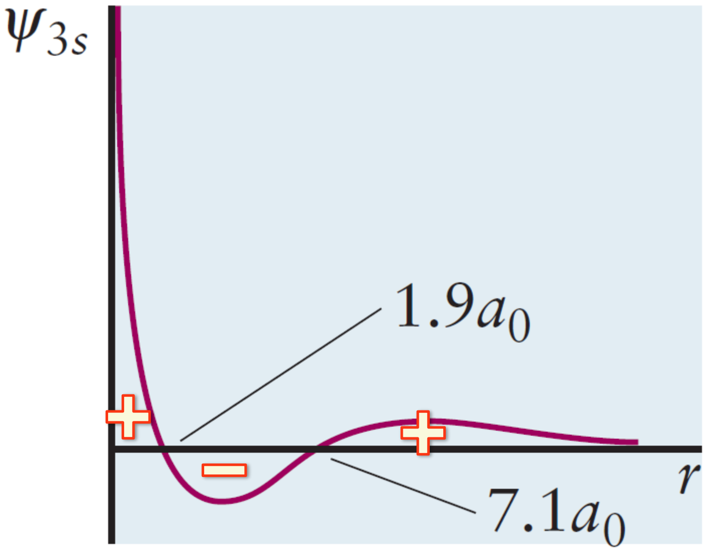
2p_x



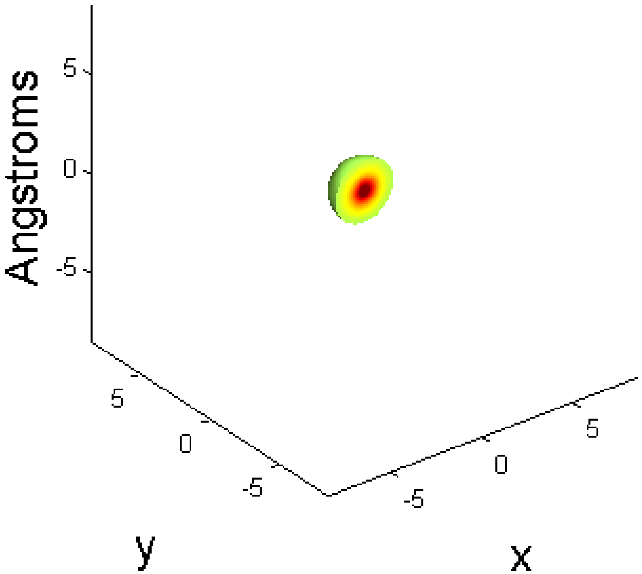
2p_y

The 3s Orbital



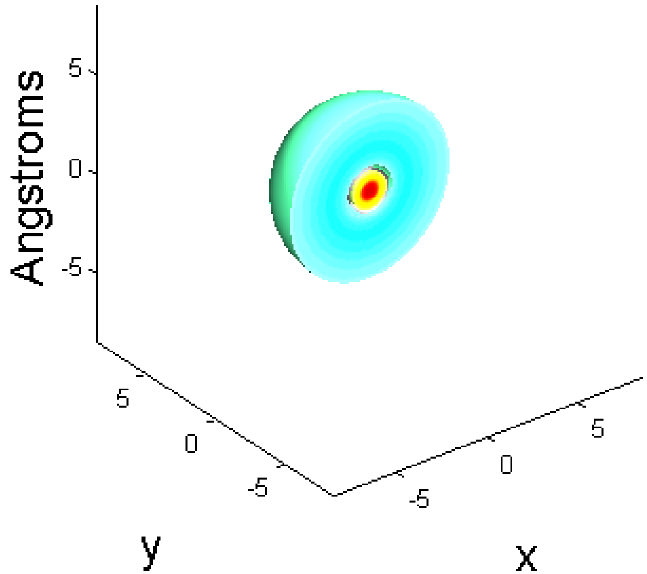


Comparison of 1*s*, 2*s*, 3*s* Orbitals



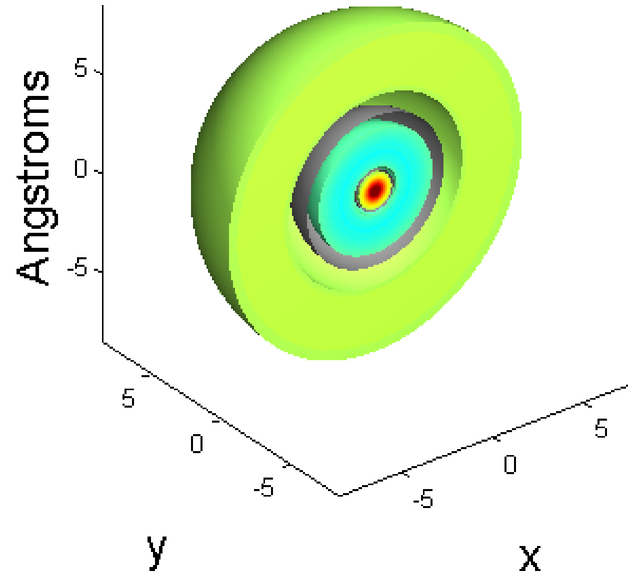
1*s*

n = 1, l = 0.



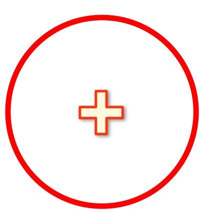
2*s*

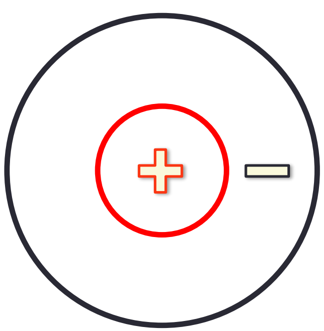
n = 2, l = 0.

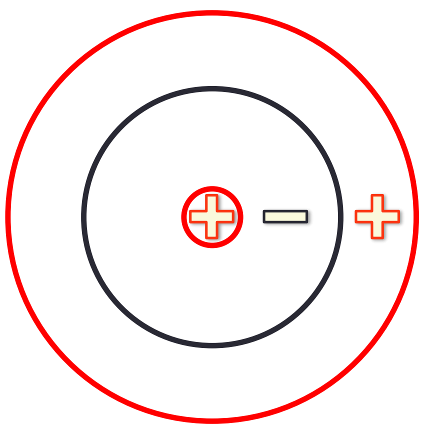


3*s*

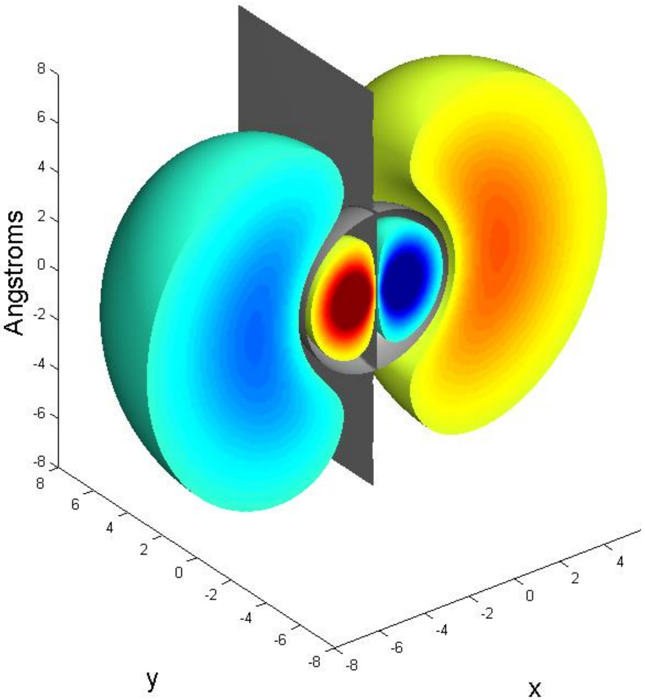
n = 3, l = 0.



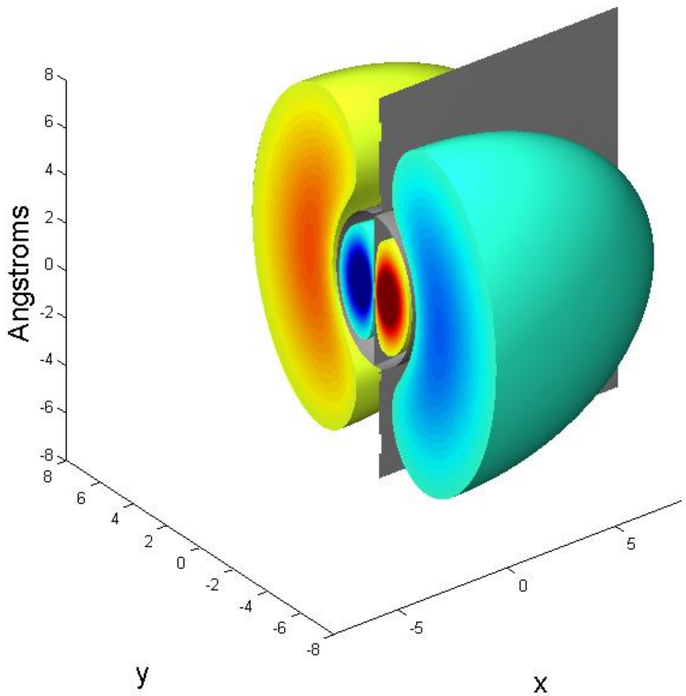




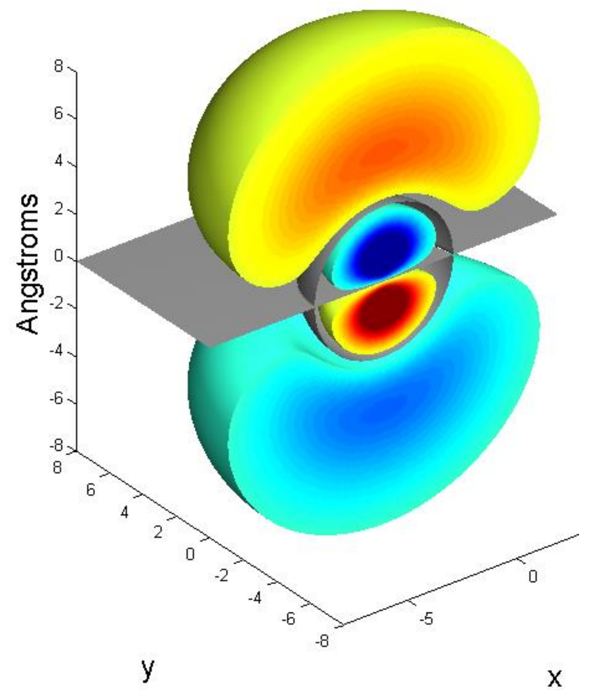
The 3*p* Orbitals



$3p_x$

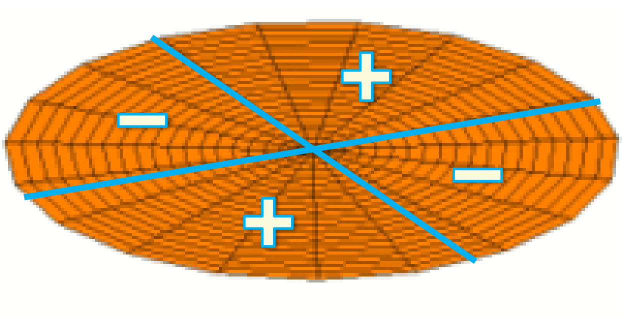


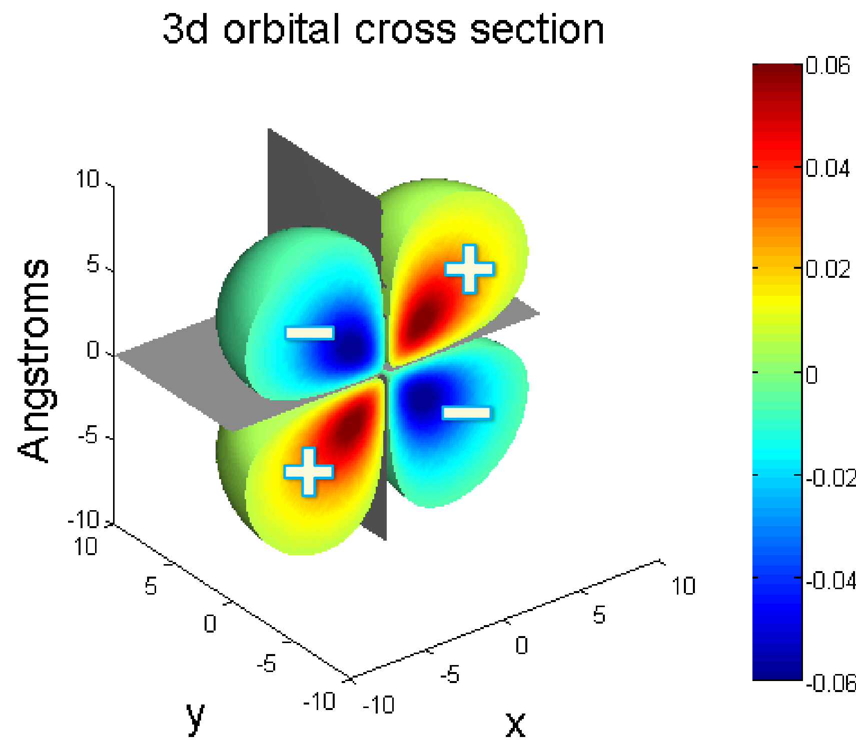
$3p_y$



$3p_z$

The 3*d* Wave in 3D

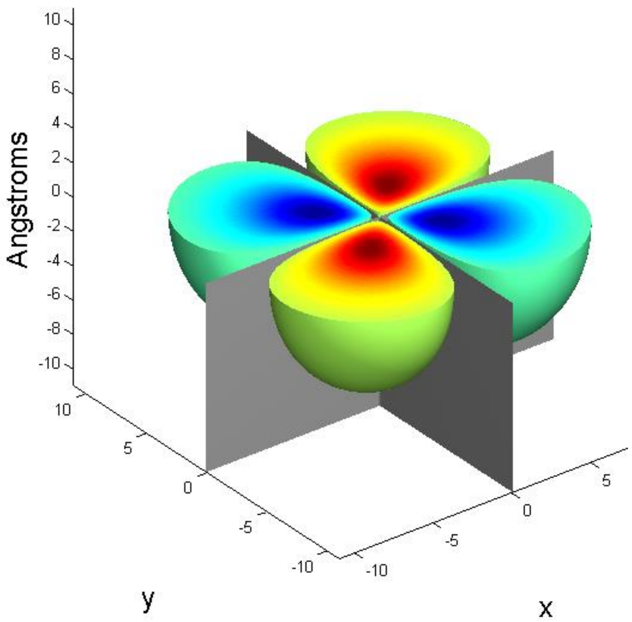




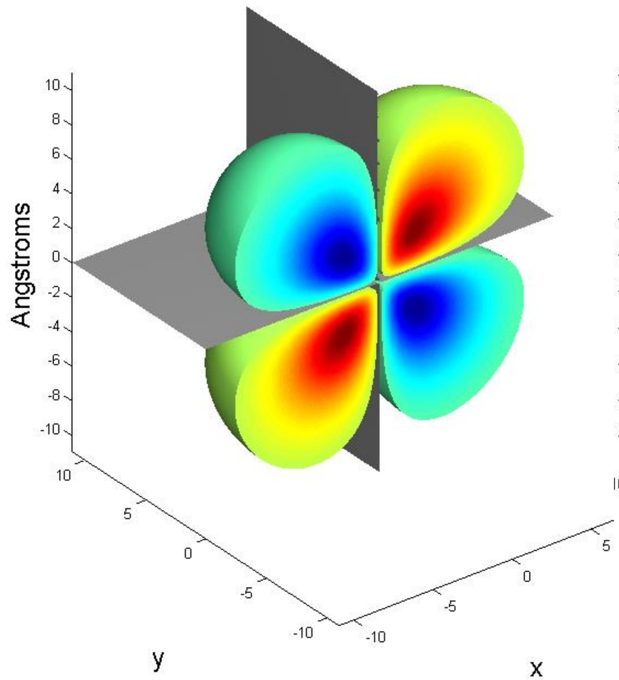
2 nodal planes (angular nodes)

$n = 3, l = 2 \implies 3d$

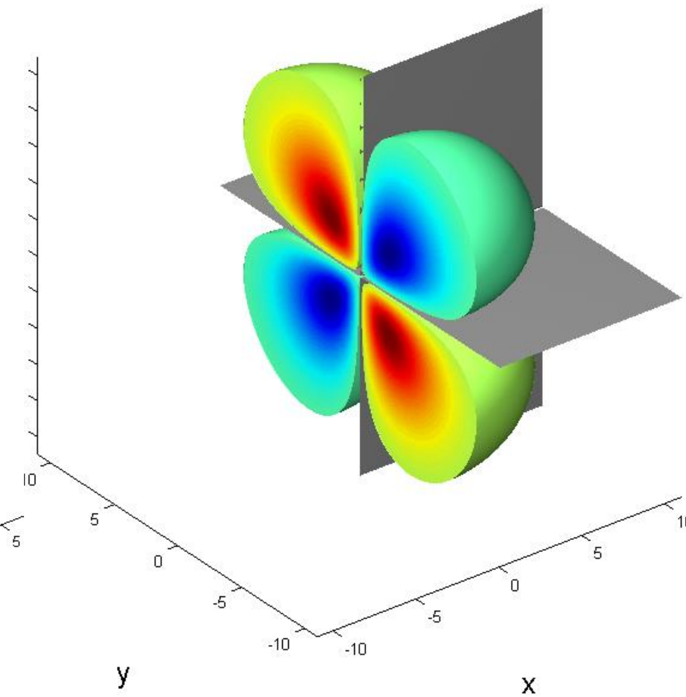
The 3*d* Orbitals (1)



$3d_{xy}$

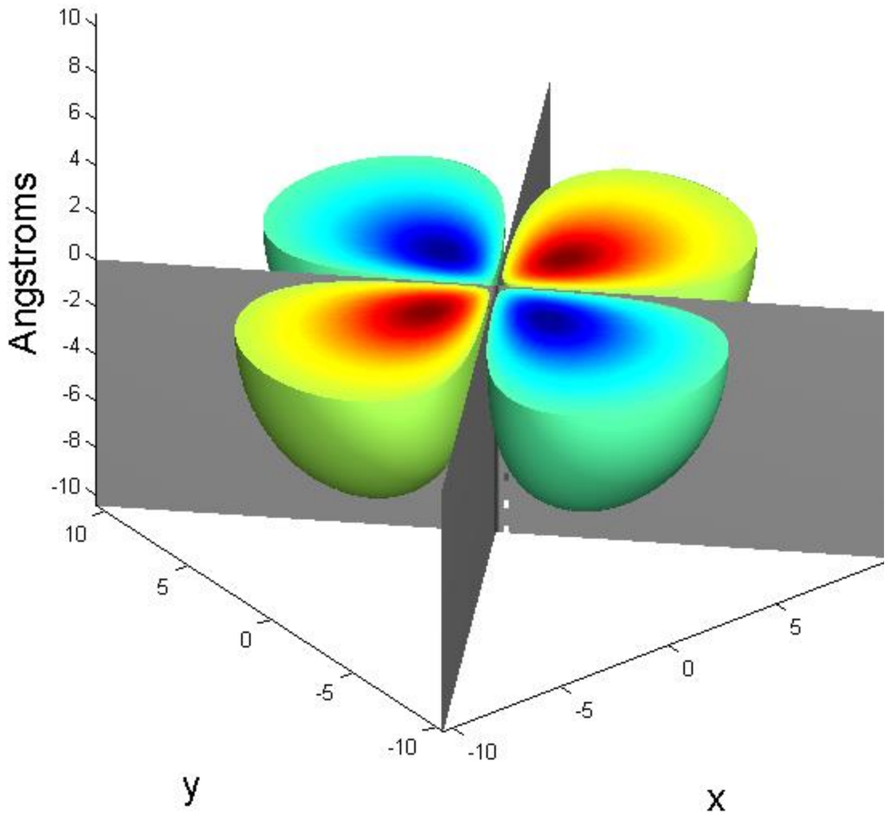


$3d_{xz}$

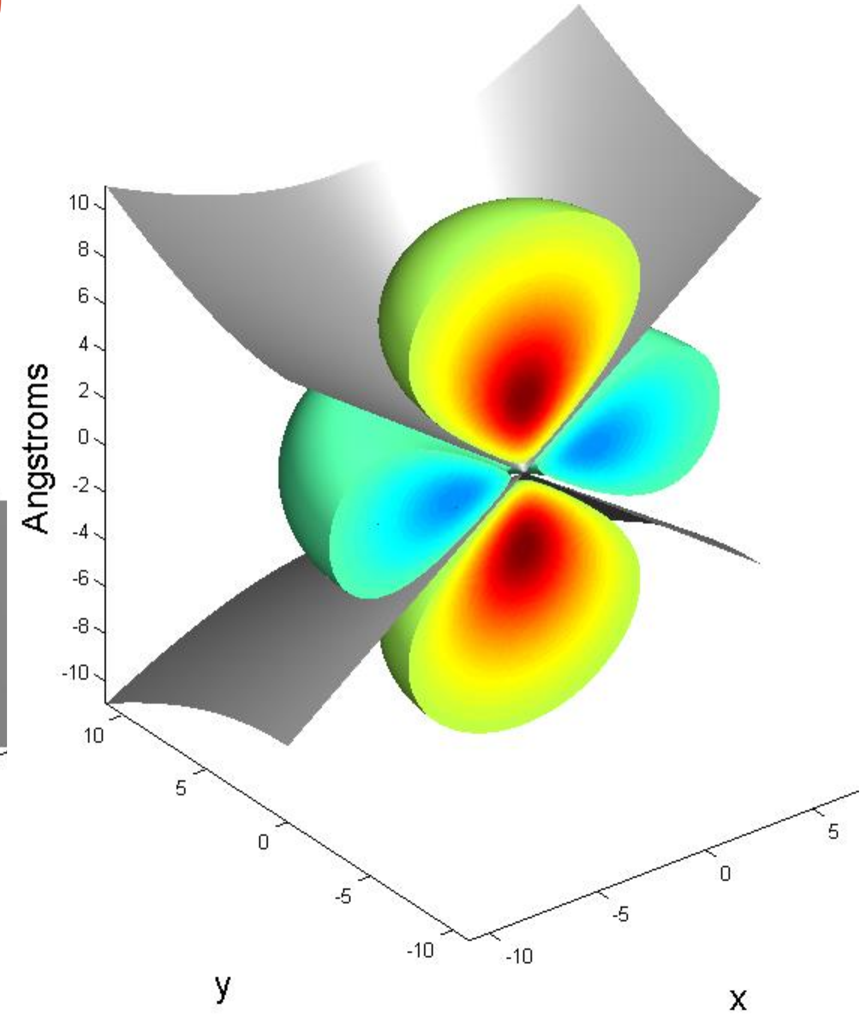


$3d_{yz}$

The 3*d* Orbitals (2)

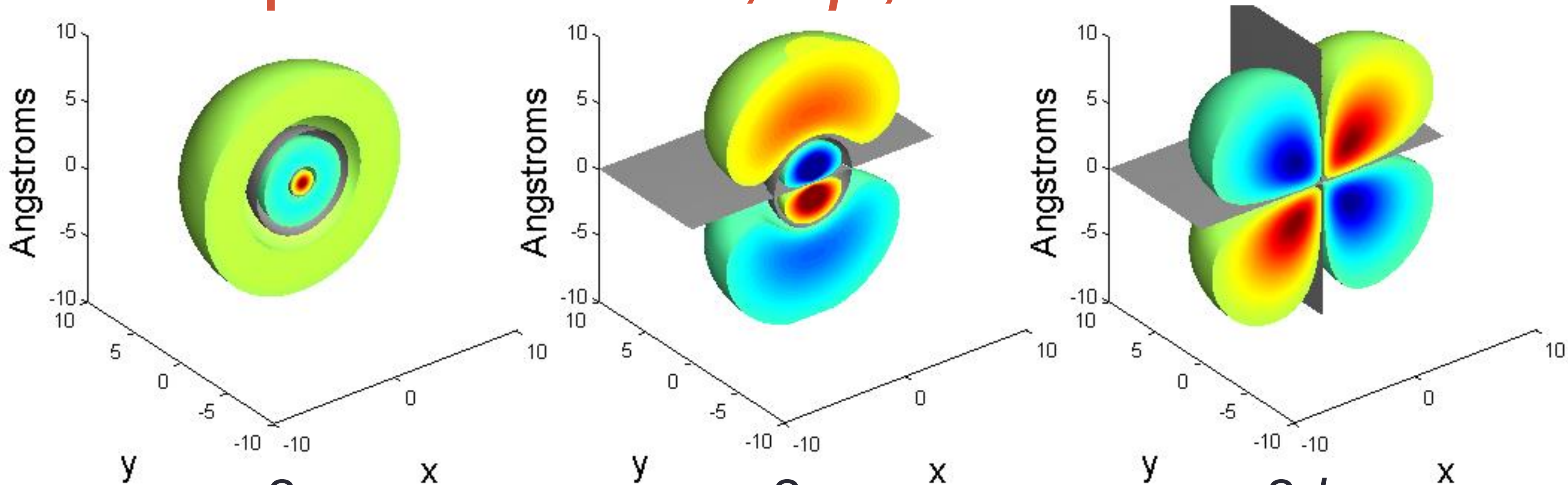


$3d_{x2-y2}$



$3d_{z2}$

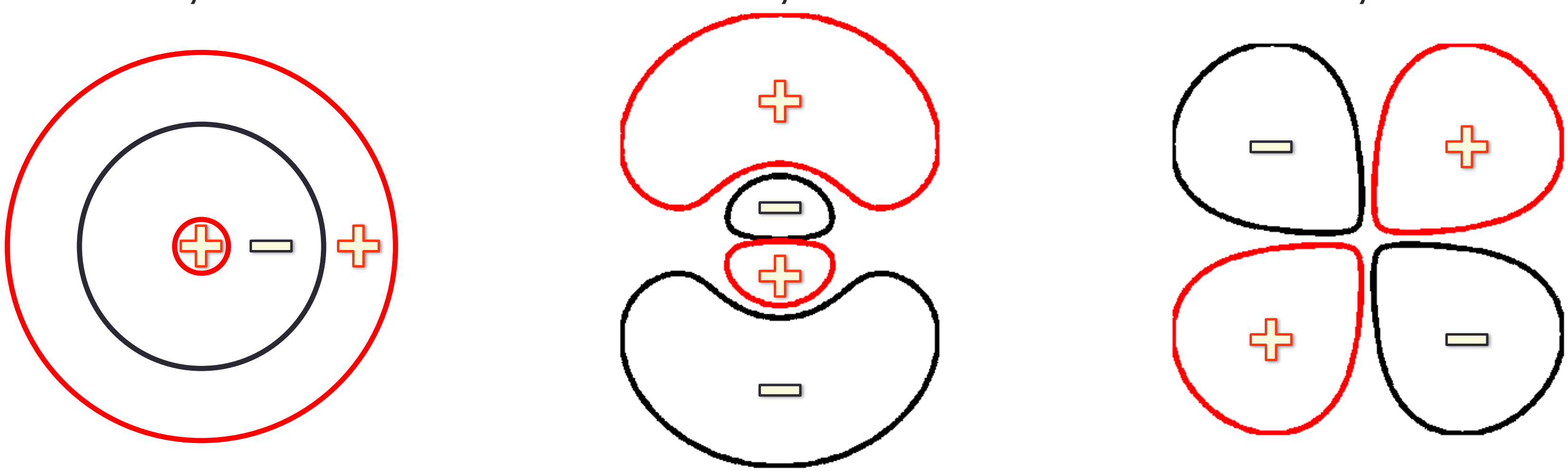
Comparison of 3*s*, 3*p*, 3*d* Orbitals



$3s$ — n = 3, l = 0.

$3p_z$ — n = 3, l = 1.

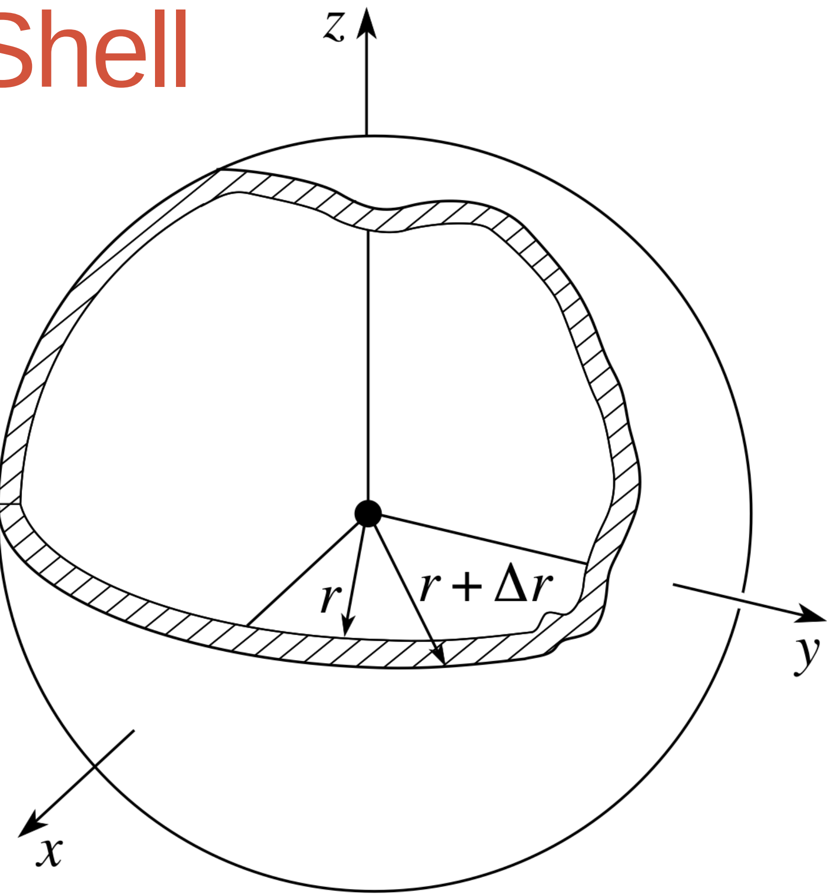
$3d_{xz}$ — n = 3, l = 2.



Outline

- Oscillations in 2D
- Atomic orbitals: Appearance
- Atomic orbitals: Properties

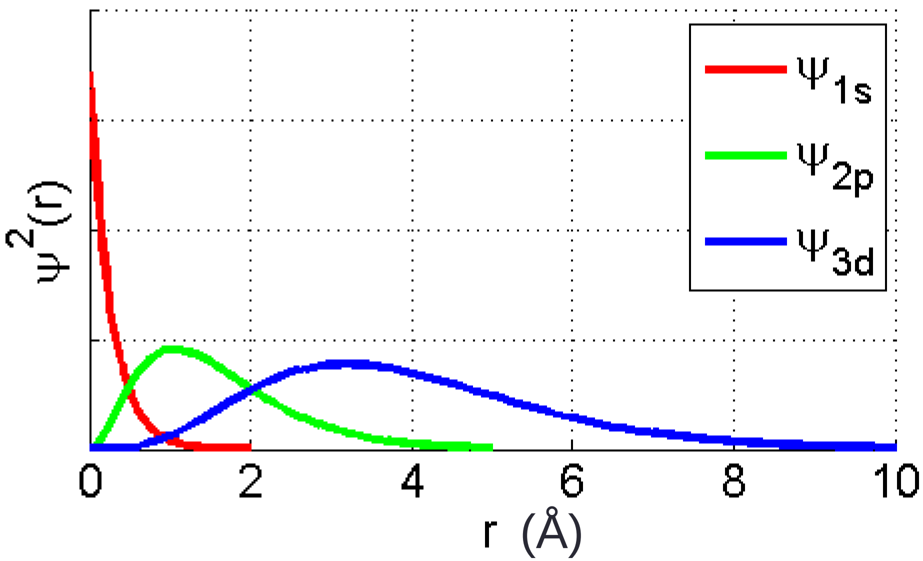
Spherical Shell

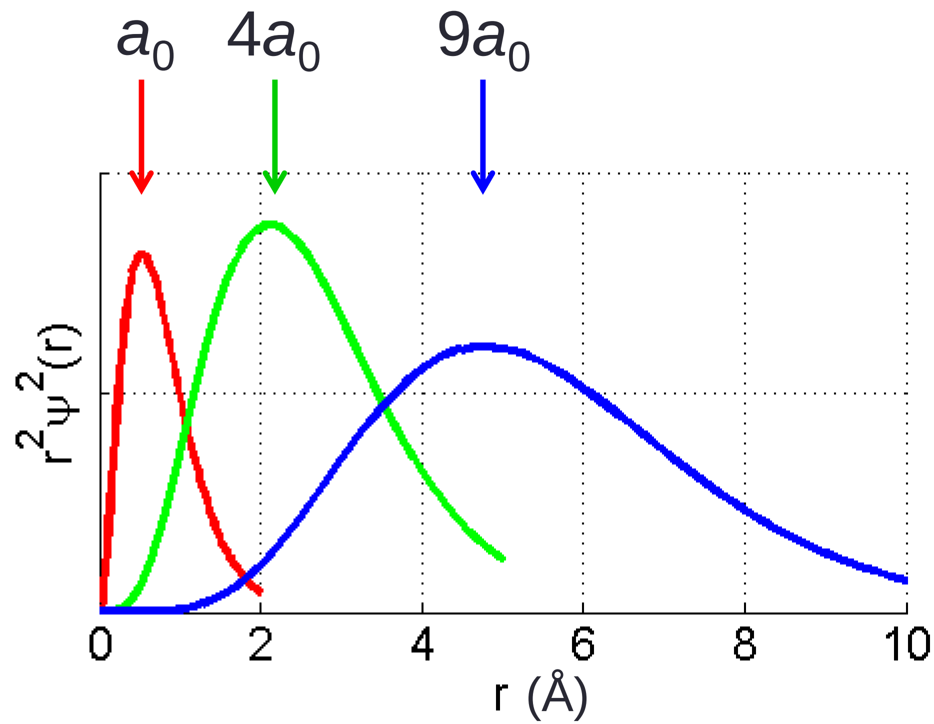


$$A = 4\pi r^2,\ dV = A dr = 4\pi r^2 dr.$$

Orbital Radius

Most probable radius r_{mp}



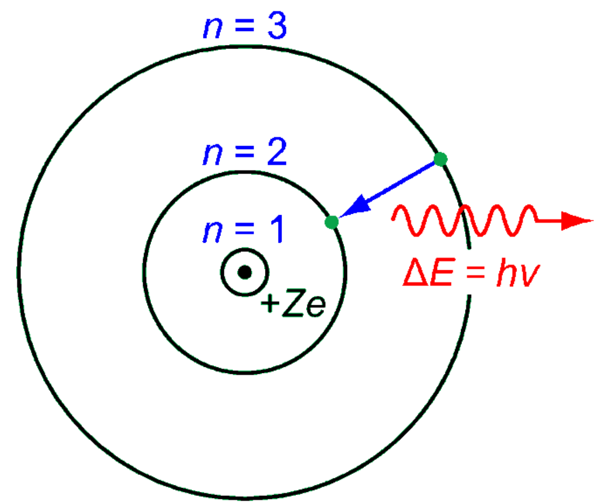


Plot $r^2\psi^2(r)$ vs. r

For Bohr Model: $r_n = n^2 a_0$
For 1*s*, 2*p*, 3*d*, …: $r_{mp,n} = n^2 a_0$

Orbital Angular Momentum

$$L = \sqrt{l(l+1)} \cdot h/2\pi \approx l \cdot h/2\pi$$

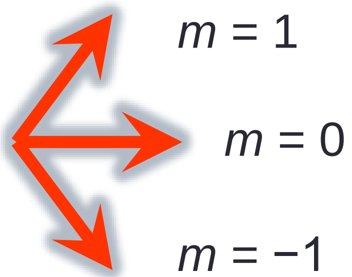


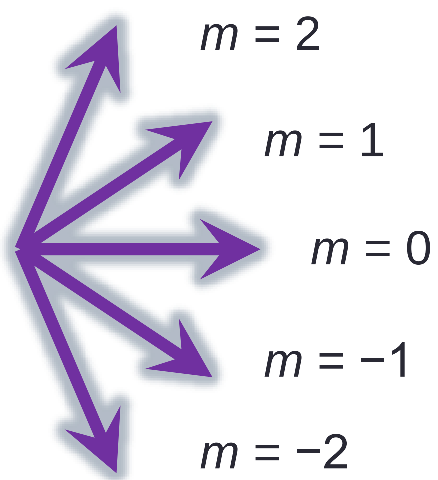
$$L_n = nh/2\pi$$

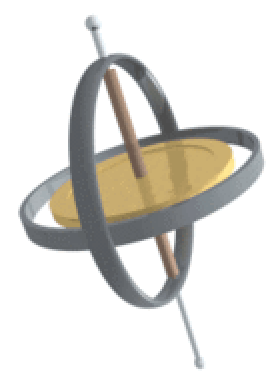
For 1*s*, 2*s* orbitals: $l = 0$, $L = 0$.

For 2*p*, 3*p* orbitals: $l = 1$, $L = \sqrt{2}\,\hbar$,
L can take 3 orientations.

For 3*d*, 4*d* orbitals: $l = 2$, $L = \sqrt{6}\,\hbar$,
L can take 5 orientations.







Old *vs*. New Quantum Theory

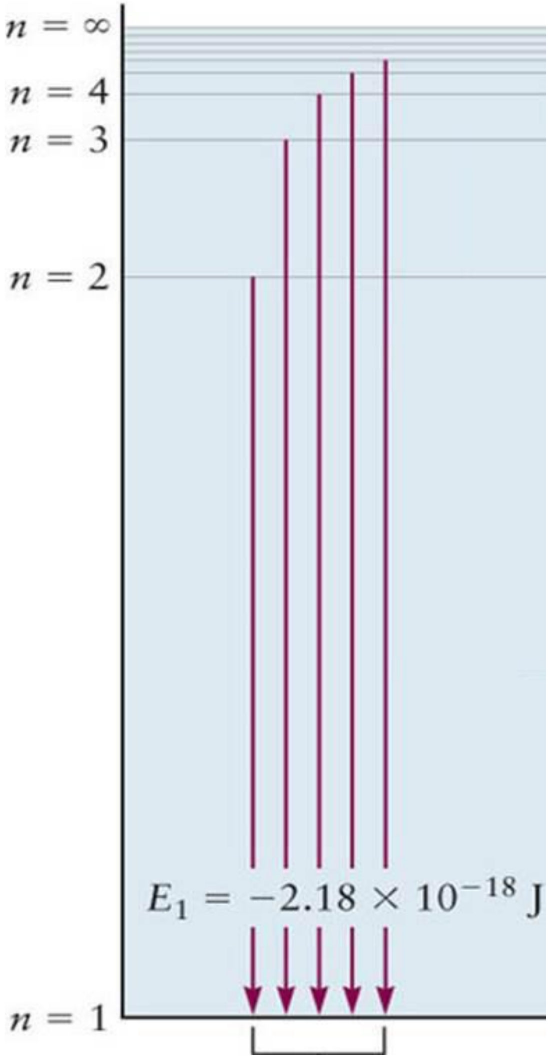
Niels Bohr
(Copenhagen, Cambridge,
1885–1962)

VS

Erwin Schrödinger
(Zürich, 1887–1961)

Orbital Energy

Bohr, OGB8 p.143

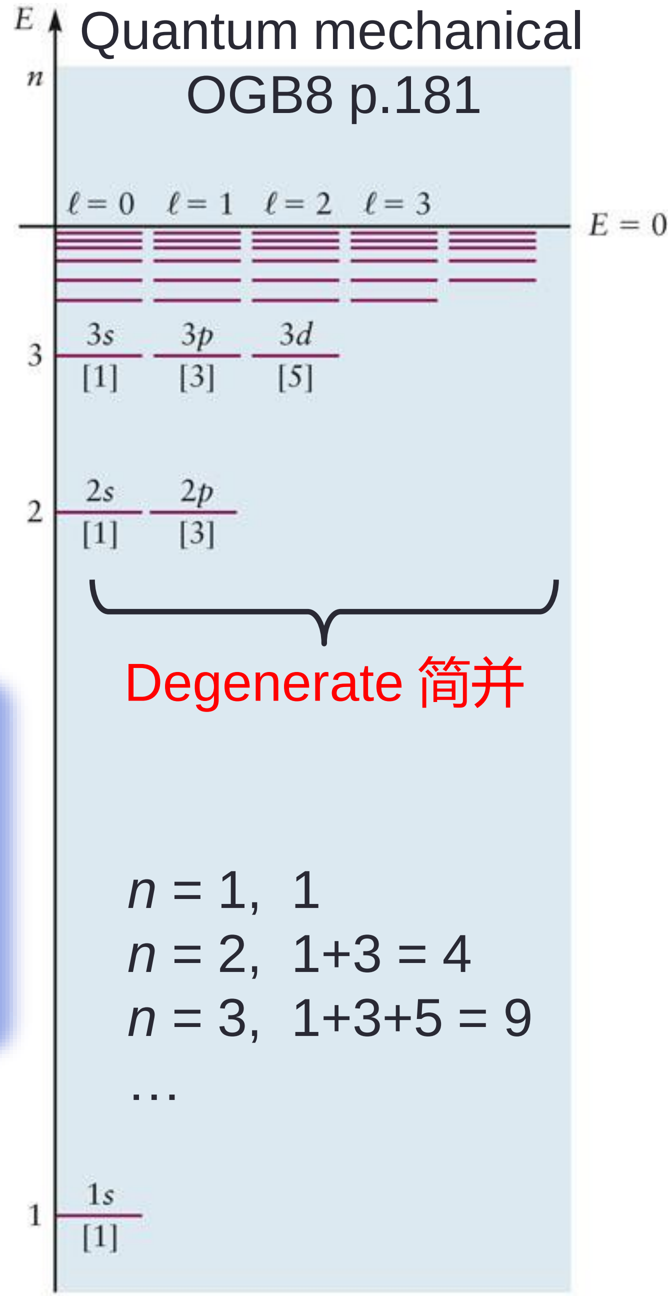


$$E_n = -\frac{R_H}{n^2},$$

$$R_H = 2.18\times10^{-18}\ \text{J}$$

$$= 13.6\ \text{eV}$$

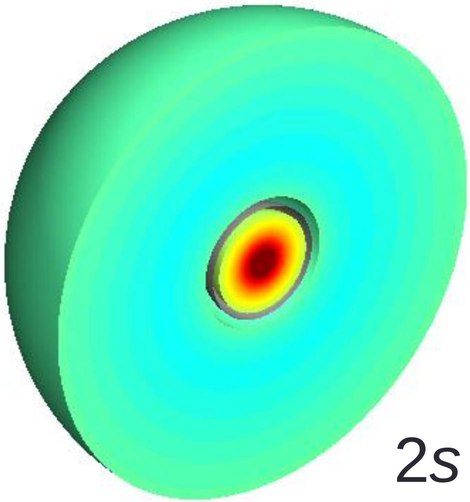
Quantum mechanical OGB8 p.181



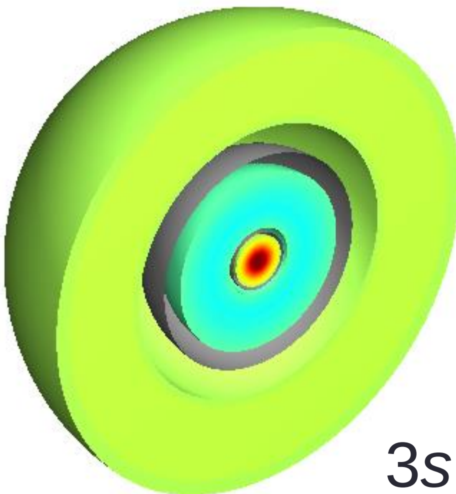
Degenerate 简并

n = 1, 1
n = 2, 1+3 = 4
n = 3, 1+3+5 = 9
…

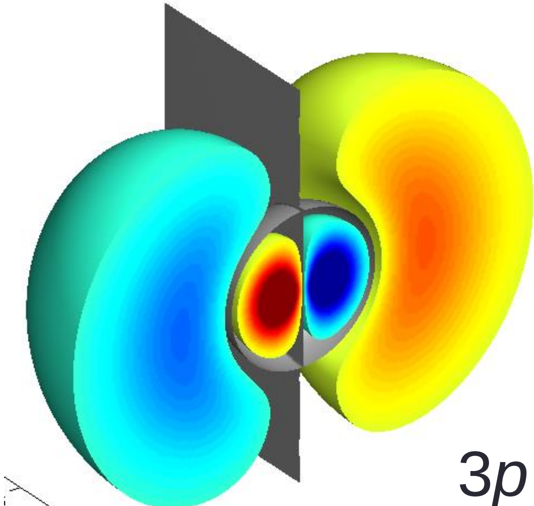
Non-Bohr Orbitals



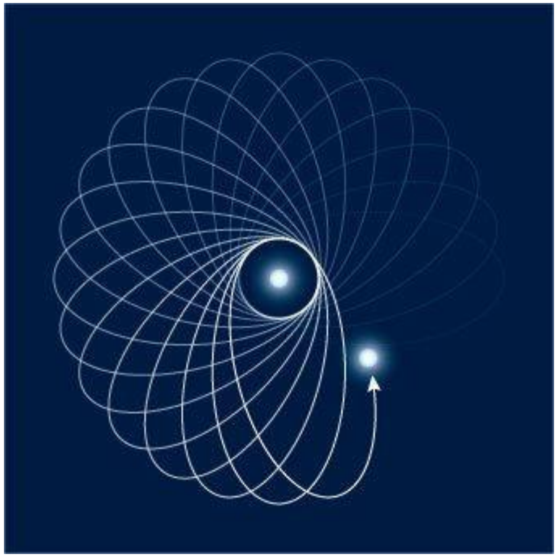
2*s*



3*s*

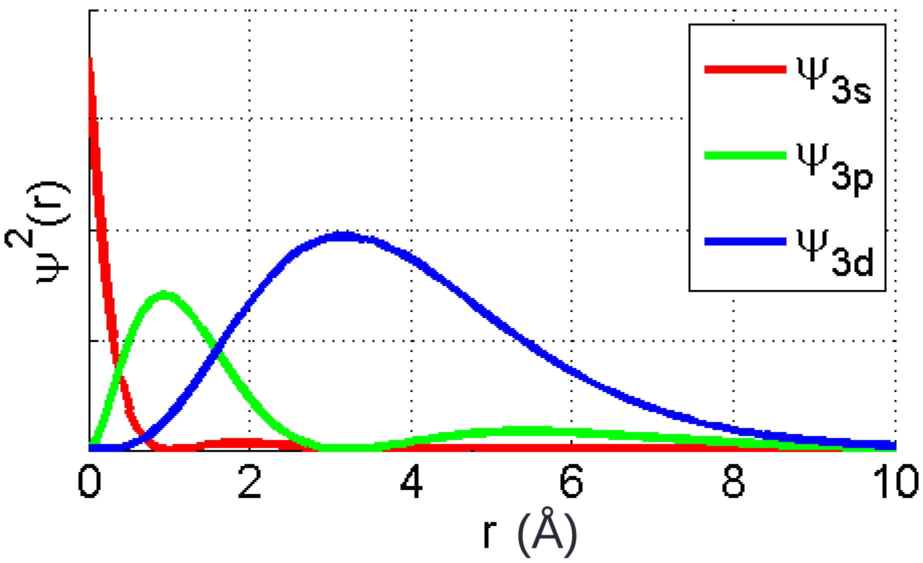


3*p*

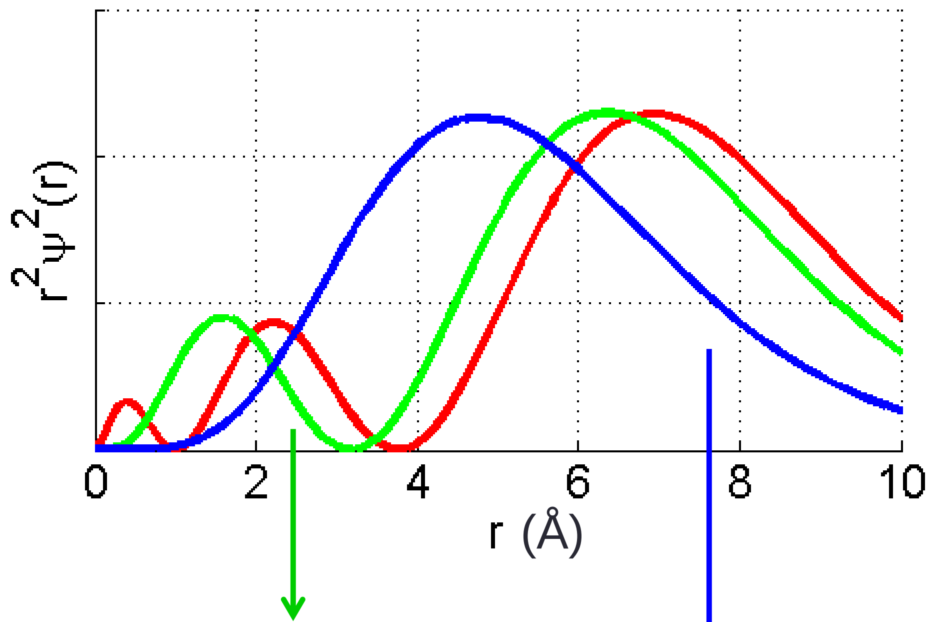


Elliptical orbits
椭圆轨道

Radial Distribution



Penetration effect 钻穿效应

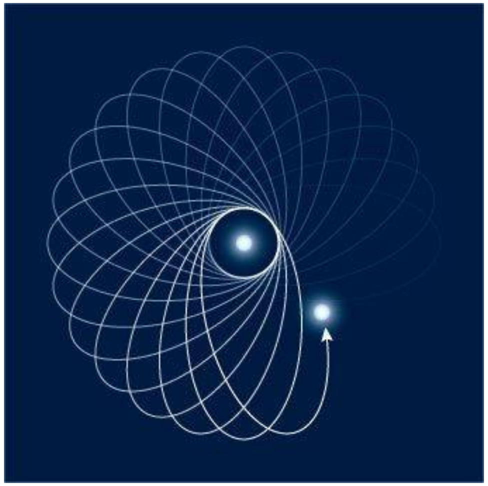


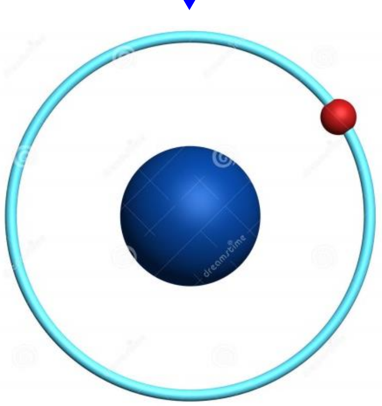
For H atom,

$r(3s) \neq r(3p) \neq r(3d)$

$E_k(3s) = E_k(3p) = E_k(3d)$

$E_p(3s) = E_p(3p) = E_p(3d)$





Summary

Principal quantum number n = Total number of nodes + 1

n = 1, 2, 3, …

Angular momentum quantum number l = Number of nodal planes

l = 0, 1, 2, …, $n - 1$.

$$E_n = -\frac{13.6\ \text{eV}}{n^2}$$

$$L = \sqrt{l(l+1)} \cdot h/2\pi \approx l \cdot h/2\pi$$

For 1*s*, 2*p*, 3*d*, …: $r_{\text{mp},n} = n^2 a_0$

2*s*, 3*s*, 2*p* exhibit penetration effect.

Midterm 1 on Wednesday Oct. 31st

Time: 10:15 – 11:00 am