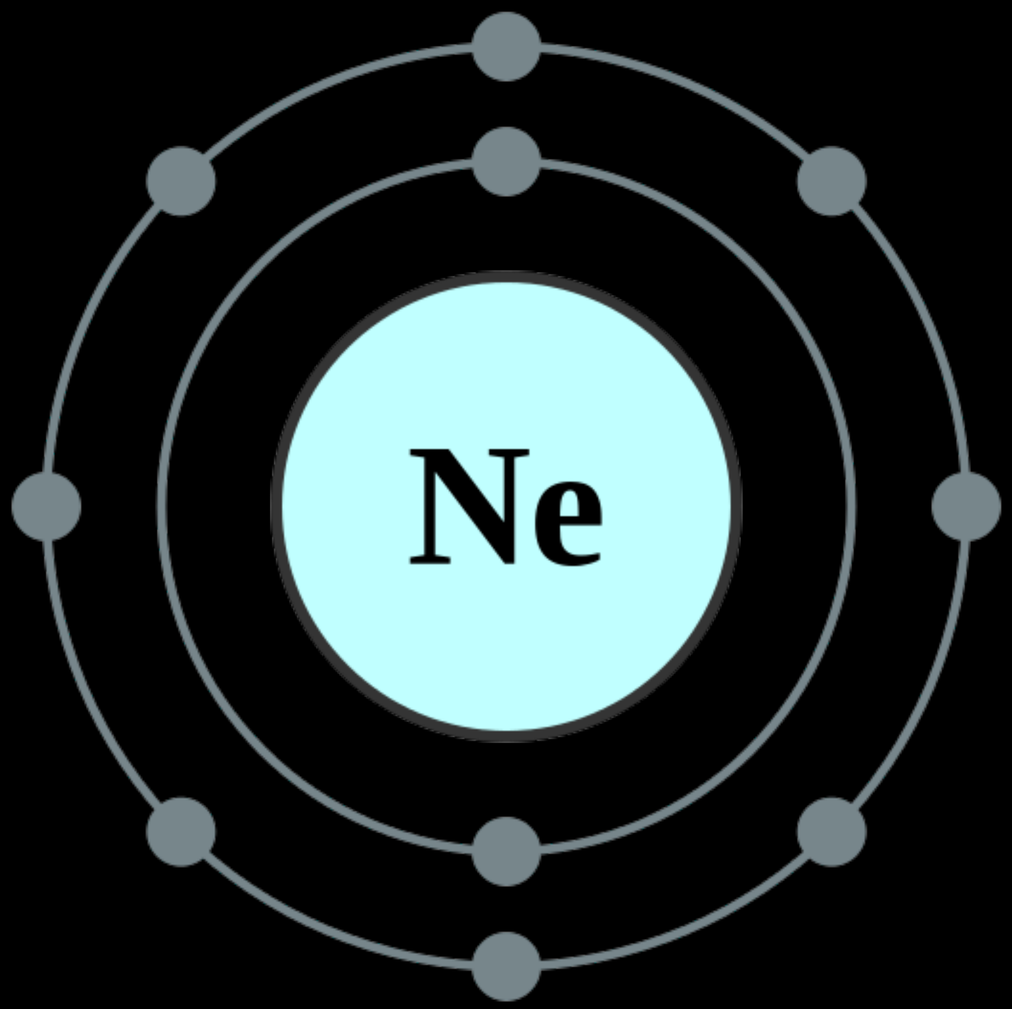
Quantum Mechanical Model

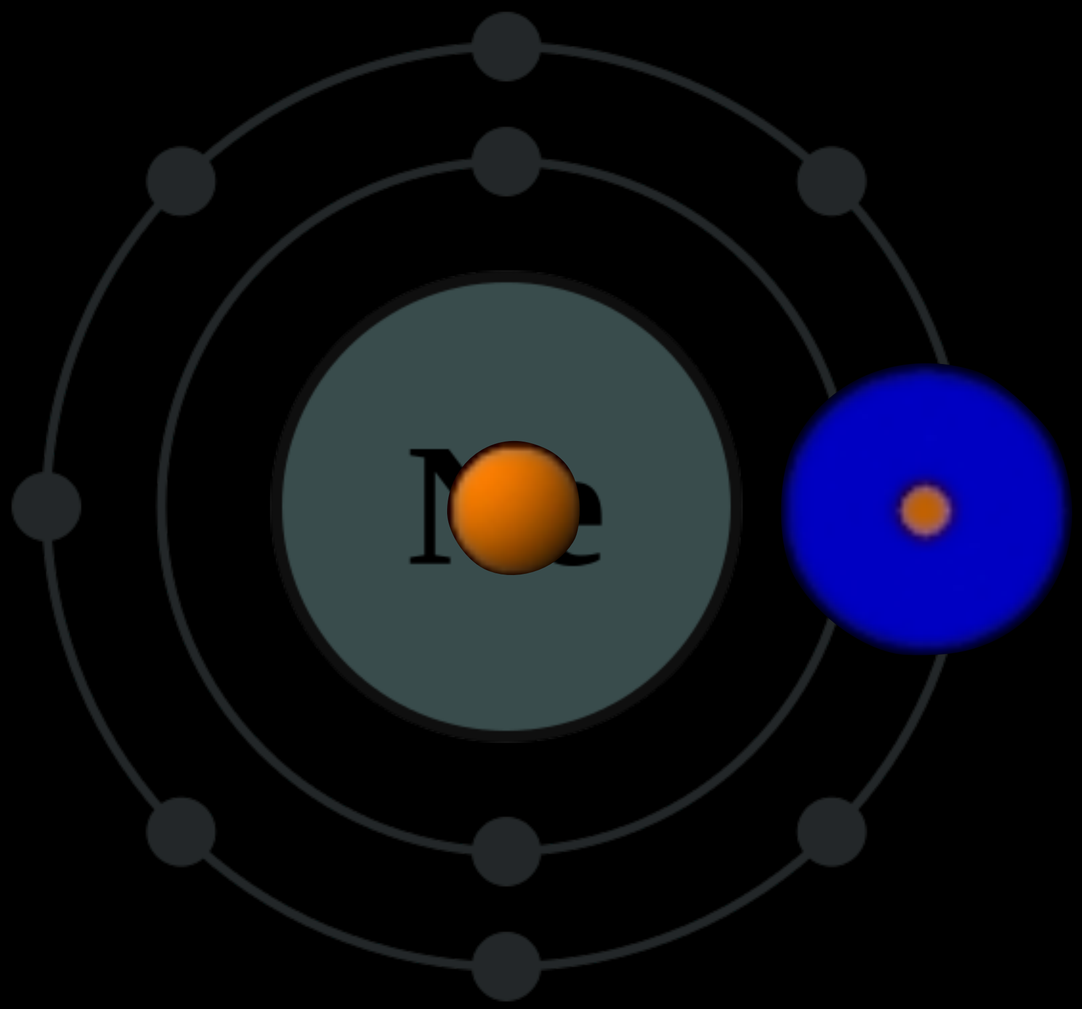
Shell Model

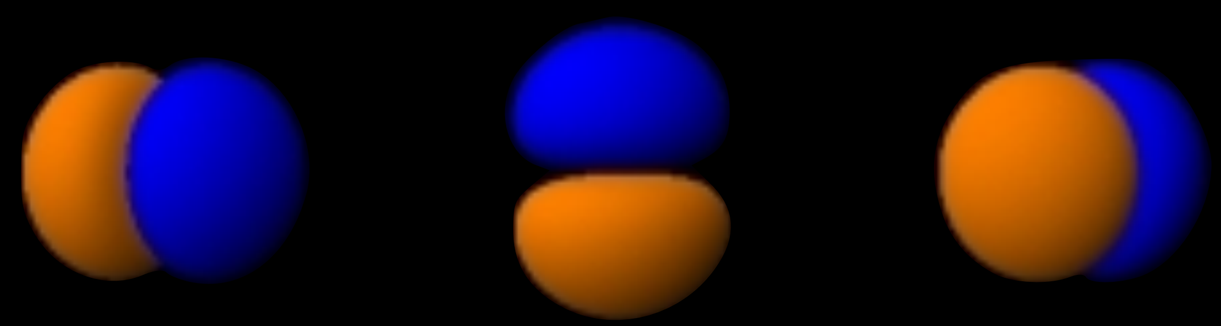


Chemistry Essentials - 007

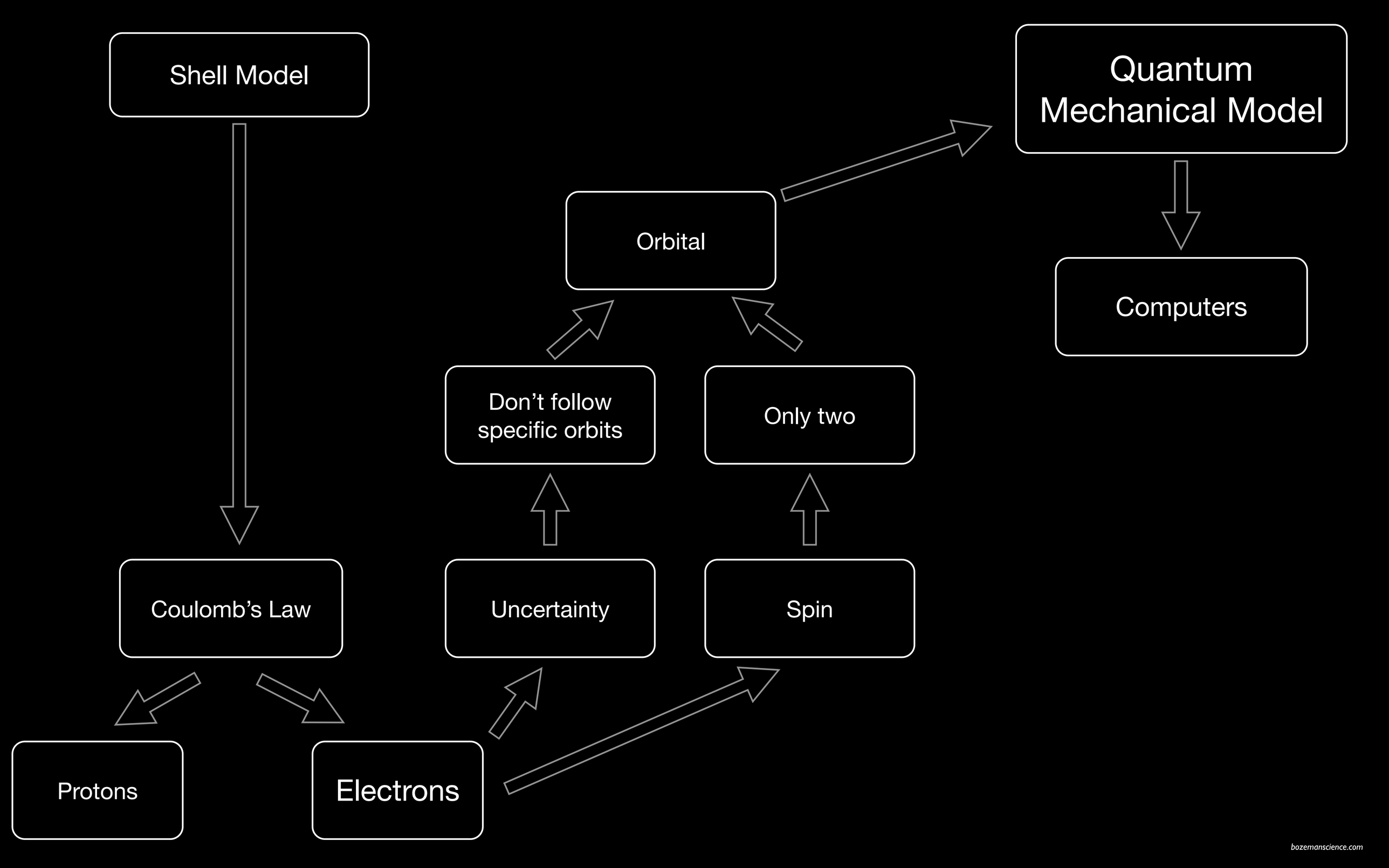
Quantum Mechanical Model

Quantum Mechanical Model





Chemistry Essentials - 007


Shell Model
Quantum Mechanical Model
Orbital
Computers
Don’t follow specific orbits
Only two
Coulomb’s Law
Uncertainty
Spin
Protons
Electrons
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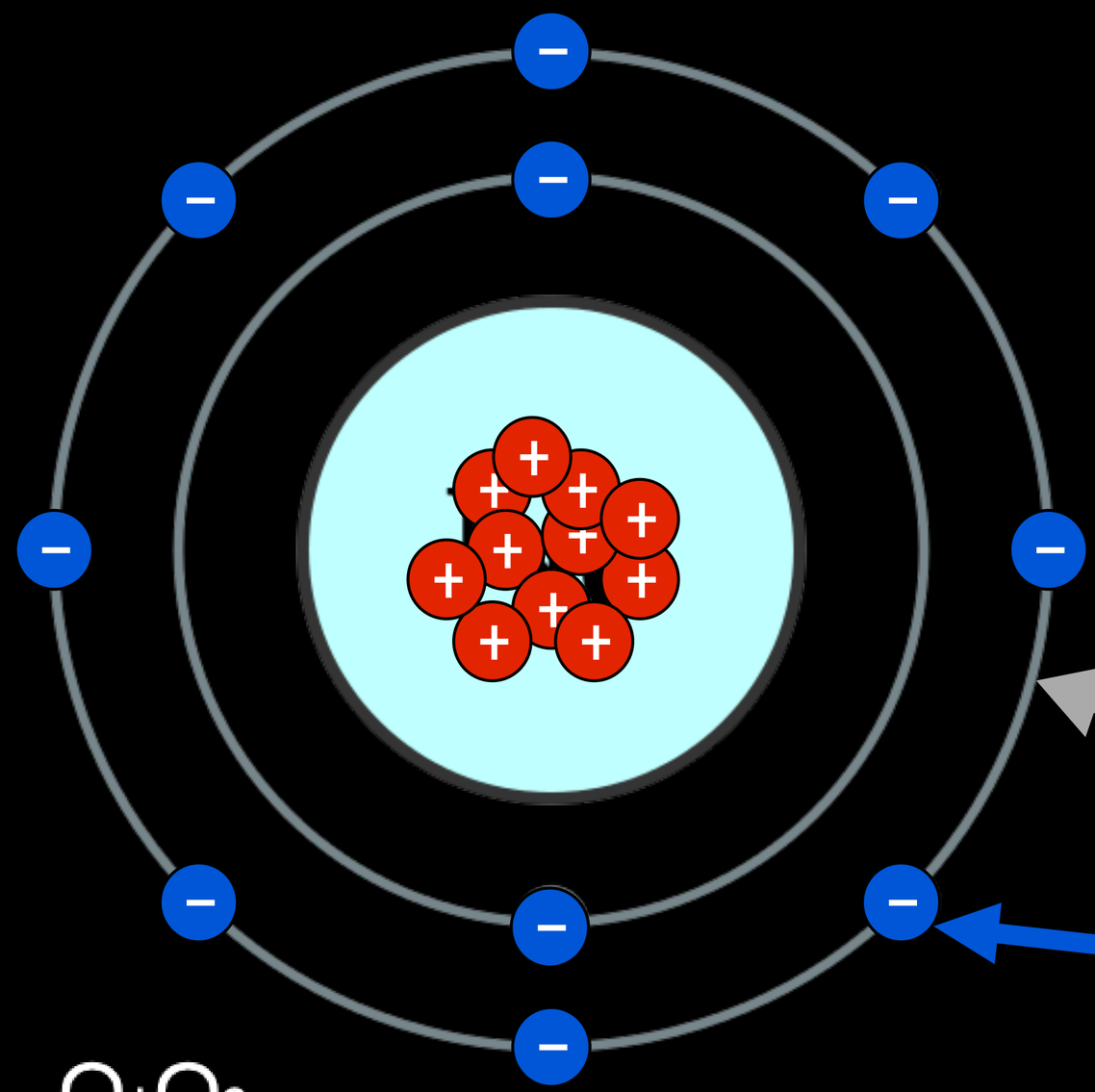
Coulomb's Law

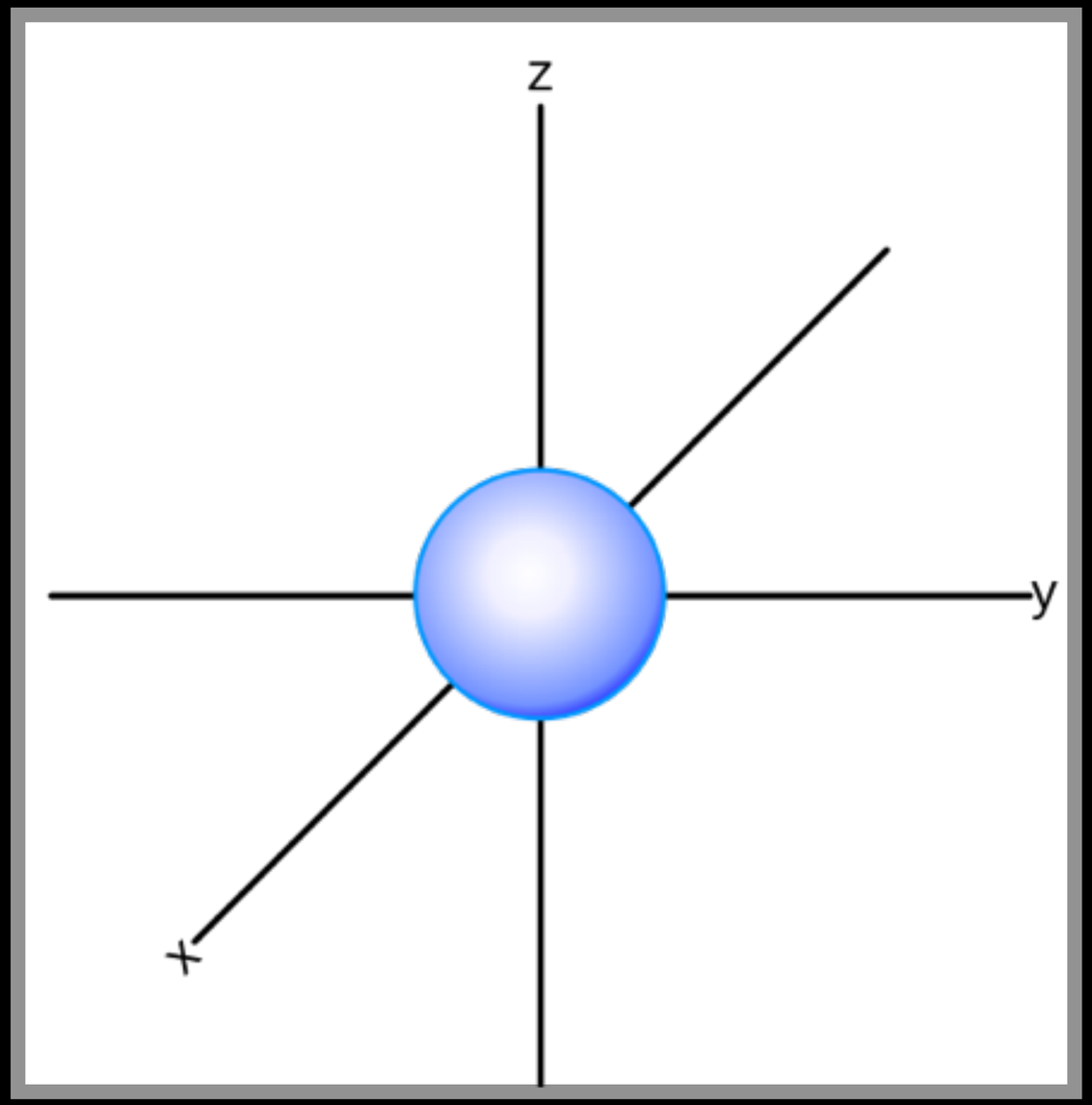


Uncertainty

Spin

$$F = k \frac{Q_1 Q_2}{r^2}$$

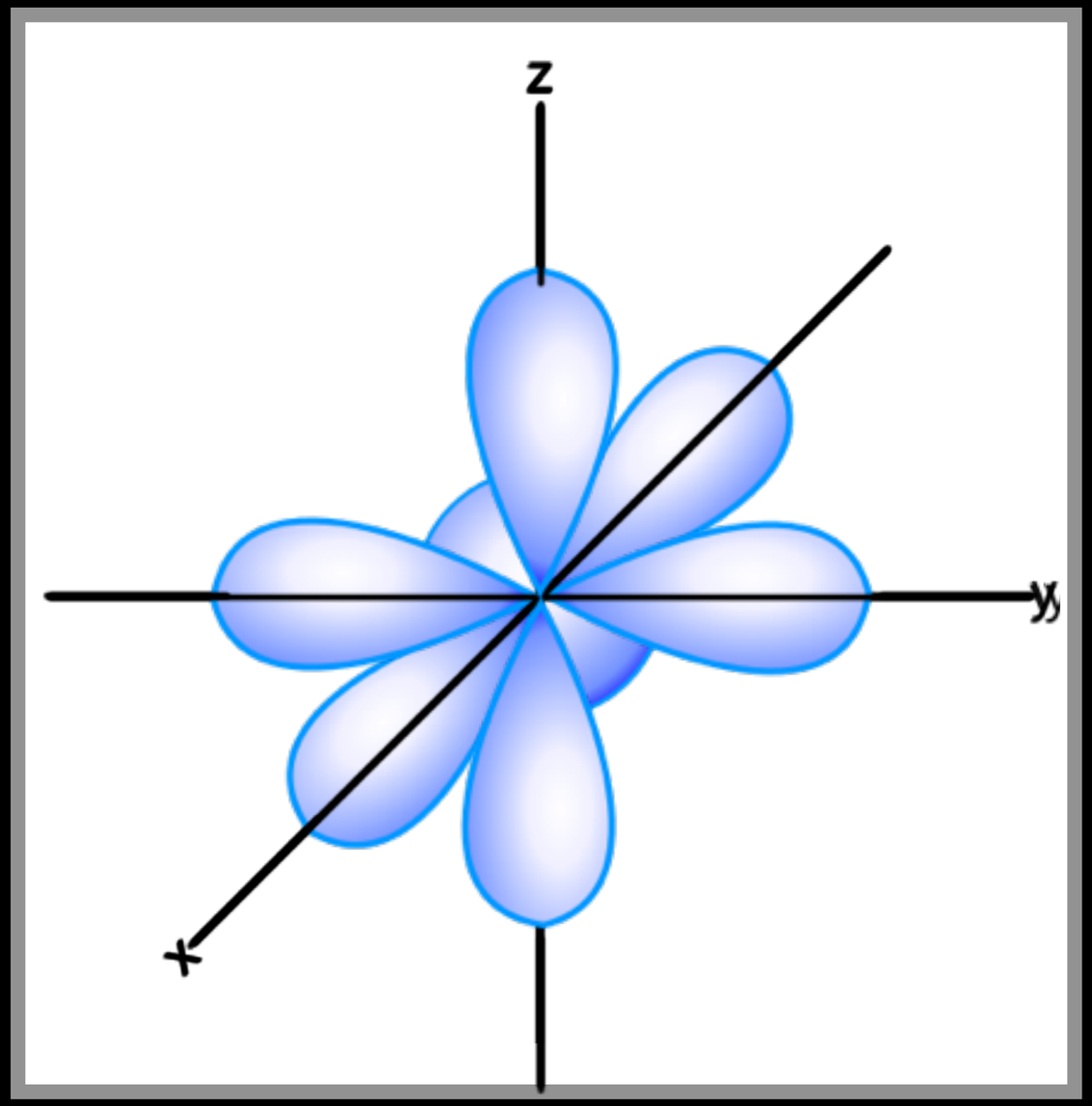
Orbitals



Uncertainty

Spin

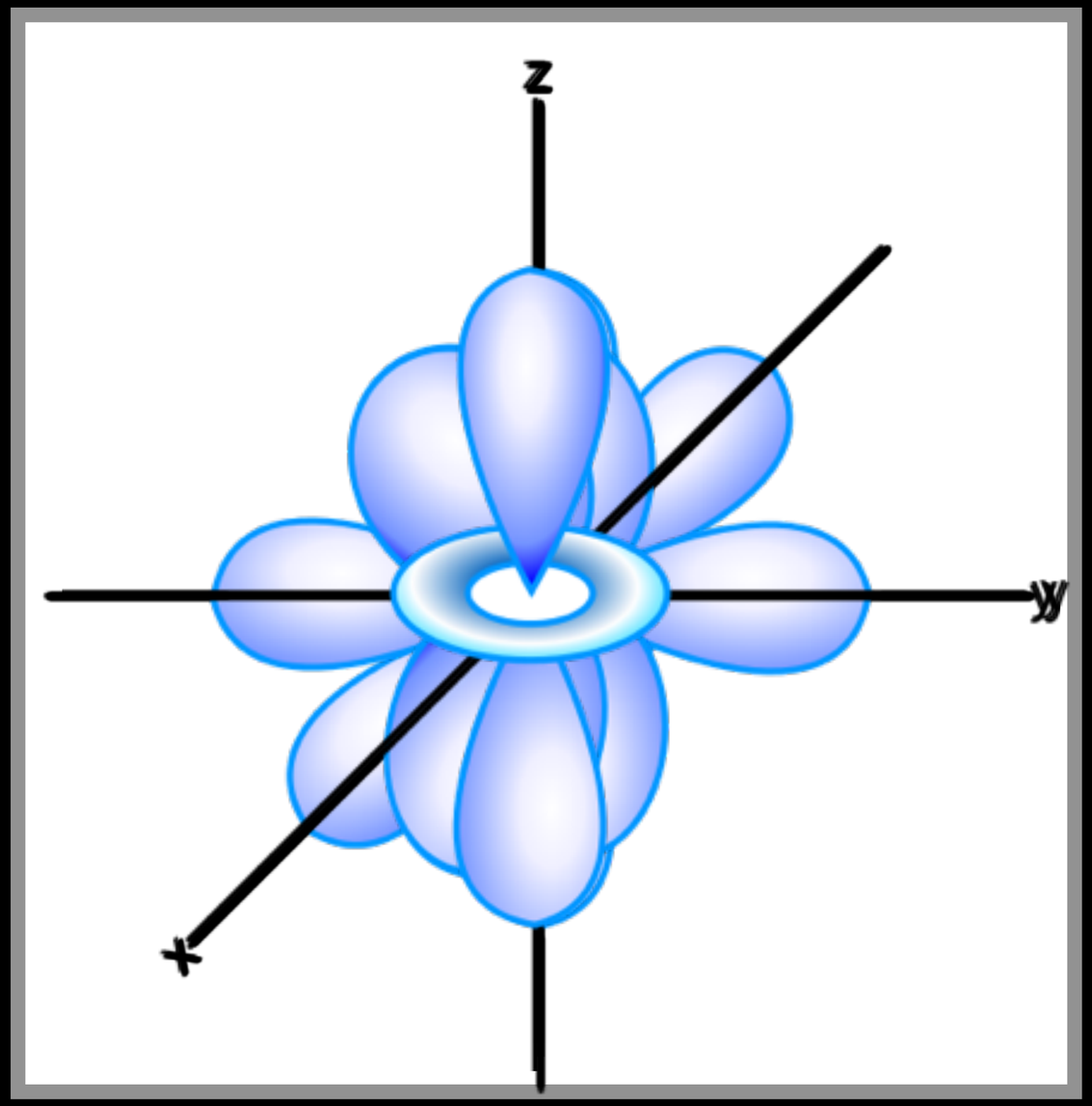
Orbitals



Uncertainty

Spin

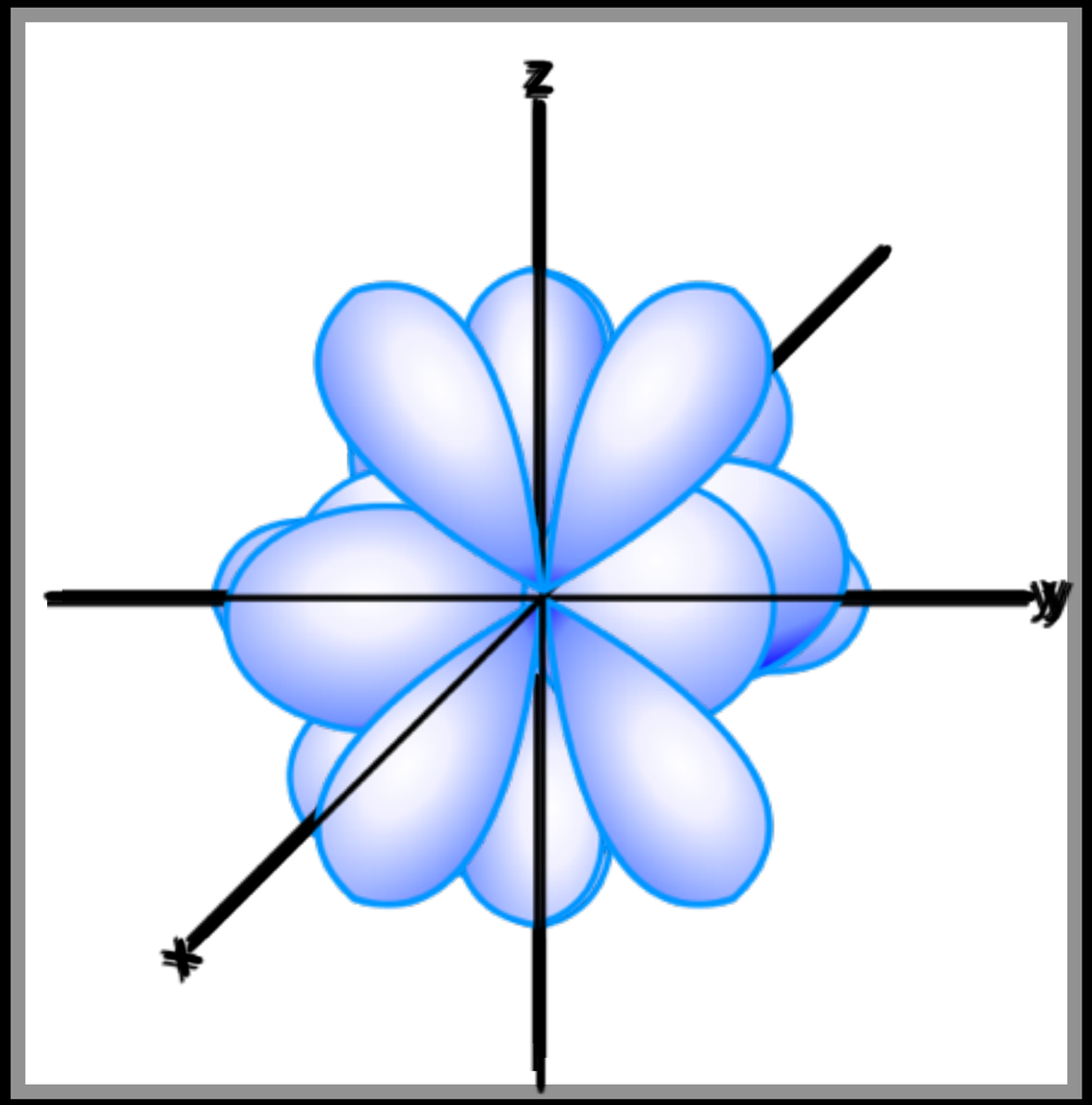
Orbitals



Uncertainty

Spin

Orbitals



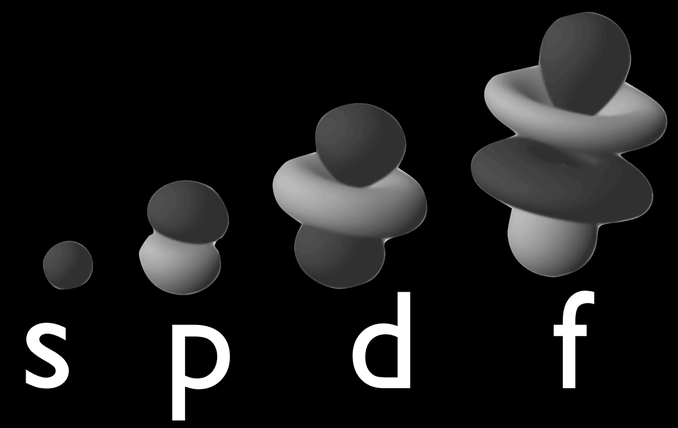
Uncertainty

Spin

Quantum Numbers

electron

size (n)				
shape (l)	s	p	d	f
orientation (m_l)	1	3	5	7
spin (m_s)	clockwise (+1/2) counter-clockwise (-1/2)			



The potential in this case is given by:

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & x \geq 0. \end{cases}$$

The solutions are superpositions of left- and right-moving waves:

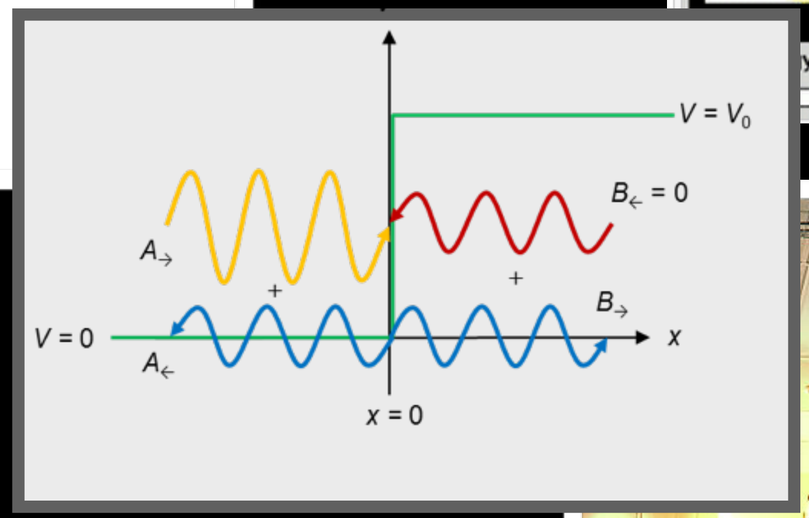
$$\psi_1(x) = \frac{1}{\sqrt{k_1}}\left(A_{\rightarrow}e^{ik_1x} + A_{\leftarrow}e^{-ik_1x}\right) \quad x < 0$$

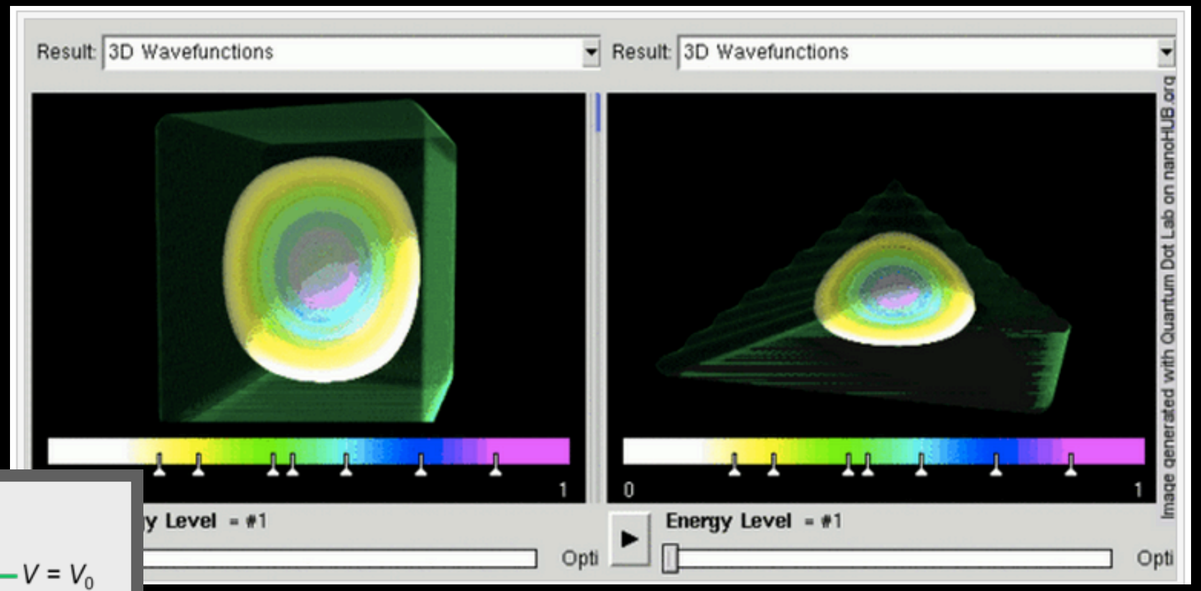
$$\psi_2(x) = \frac{1}{\sqrt{k_2}}\left(B_{\rightarrow}e^{ik_2x} + B_{\leftarrow}e^{-ik_2x}\right) \quad x > 0$$

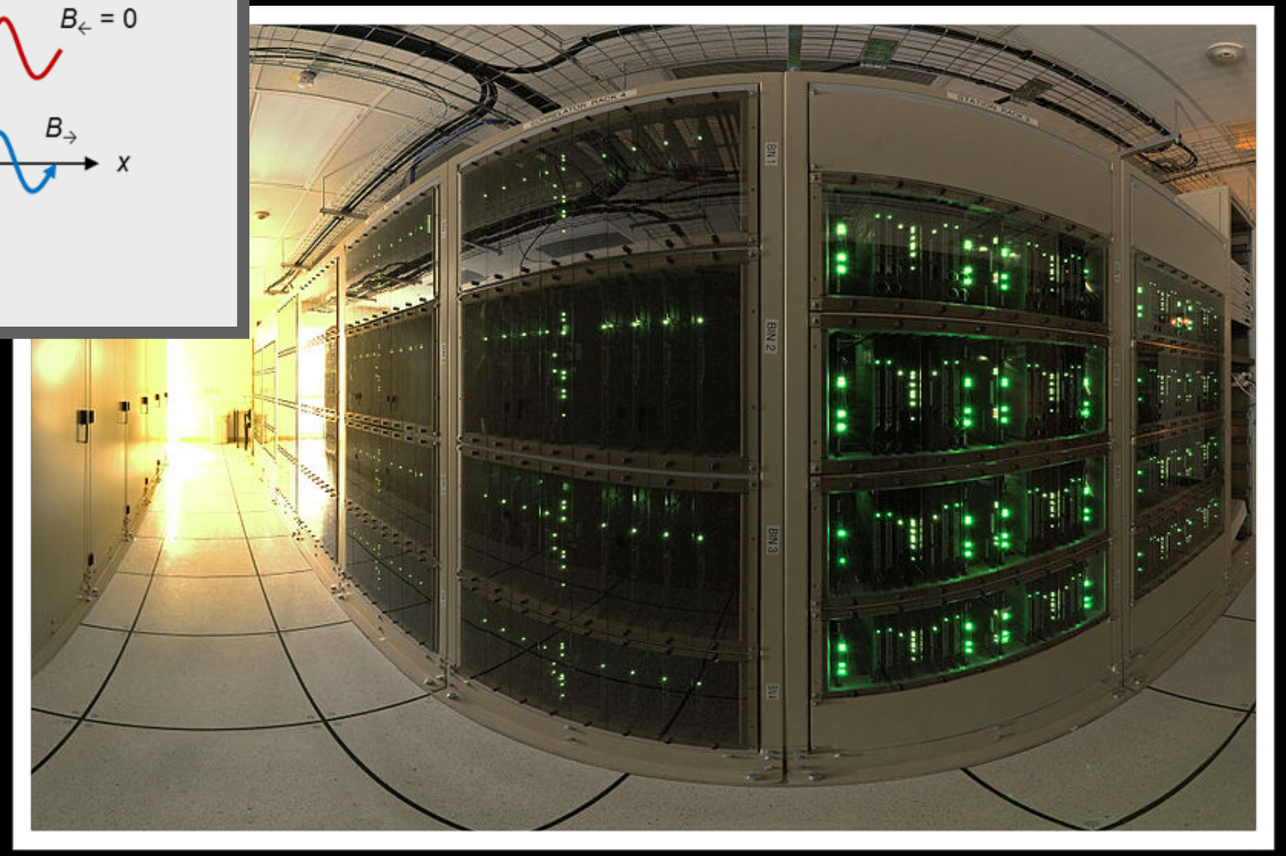
where the wave vectors are related to the energy via

$$k_1 = \sqrt{2mE/\hbar^2}, \text{ and}$$

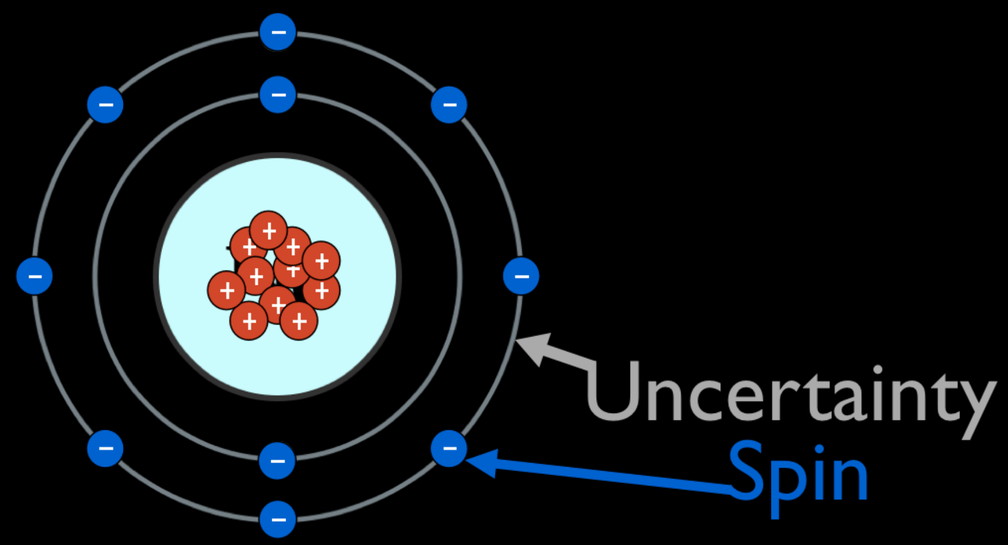
$$k_2 = \sqrt{2m(E - V_0)/\hbar^2}$$







Did you learn?



How the quantum mechanical model can refine the classical shell model.

Acknowledgements

"File:Electron Orbitals.svg," August 2, 2013. http://en.wikipedia.org/wiki/File:Electron_orbitals.svg.
"File:Electron Shell 010 Neon - No Label.svg," August 2, 2013. http://en.wikipedia.org/wiki/File:Electron_shell_010_Neon_-_no_label.svg.
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"File:IBM Blue Gene P Supercomputer.jpg," August 2, 2013. http://en.wikipedia.org/wiki/File:IBM_Blue_Gene_P_supercomputer.jpg.
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Kaluza, Tim. *Deutsch: Übersicht Der Orbitale*, *Chemie*., 2012. Own work. http://commons.wikimedia.org/wiki/File:Chemie_Orbitale.svg.
"Quantum Mechanics," August 2, 2013. http://en.wikipedia.org/w/index.php?title=Quantum_mechanics&oldid=566061324.

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