

Lecture 3. Atomic Structure

Physical Chemistry 1, Winter 2022

Department of Chemistry

Jiho Son

Seoul National University

“Classification” of atoms

Class 1. Atom with one electron (we call this *hydrogen*)

Class 2. Atom with more than one electron (we call this *multielectron atom*)

This classification is very silly, but crucial since *electron-electron repulsion* makes everything sophisticated.

Review: quantum numbers

Recall these relations you have learned in general chemistry course.

$$n = 0, 1, 2, \dots$$

$$l = 0, 1, \dots, n - 1$$

$$m = 0, \pm 1, \dots, \pm l$$

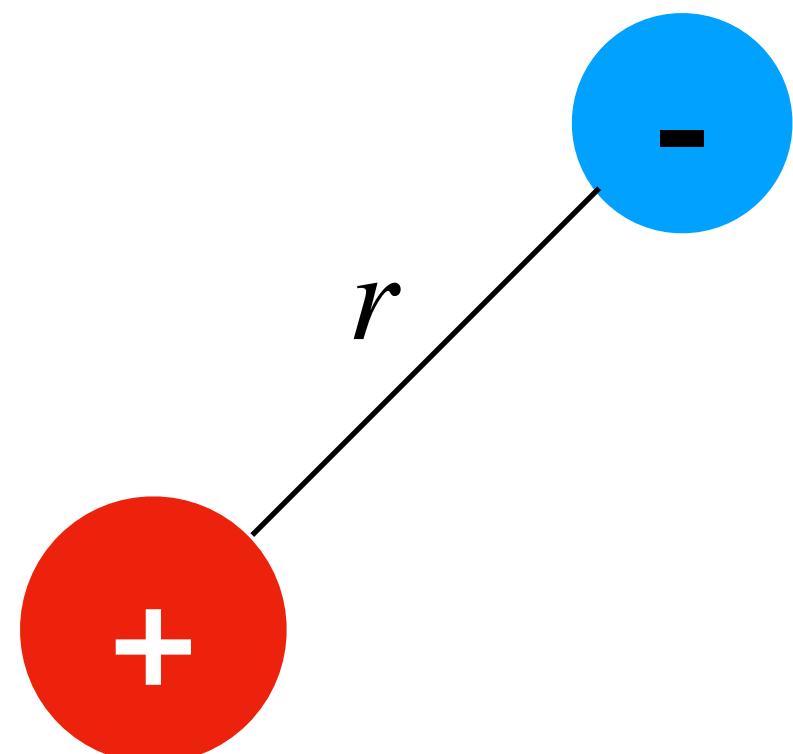
$$m_s = \pm \frac{1}{2}$$

Quantum numbers (excluding spin) arise while you solve the Schrödinger equation of hydrogen atom.

Hamiltonian of Hydrogen atom

Recall that Hamiltonian is sum of kinetic and potential energy. Electric potential term here.

Charge of a proton and an electron are $+e$ and $-e$, respectively.



$$\hat{H} = -\frac{\hbar^2}{2M} \nabla'^2 - \frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r}$$

where M and m are masses of proton and electron, respectively.

Primed Laplacian correspond to the differentiation respect to nuclear coordinate.

Born-Oppenheimer Approximation

However, a proton is $\sim 1,836$ times heavier than an electron. Therefore, we can neglect the motion of nucleus - fix the nucleus at the origin, and only consider the motion of nucleus.

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r}$$

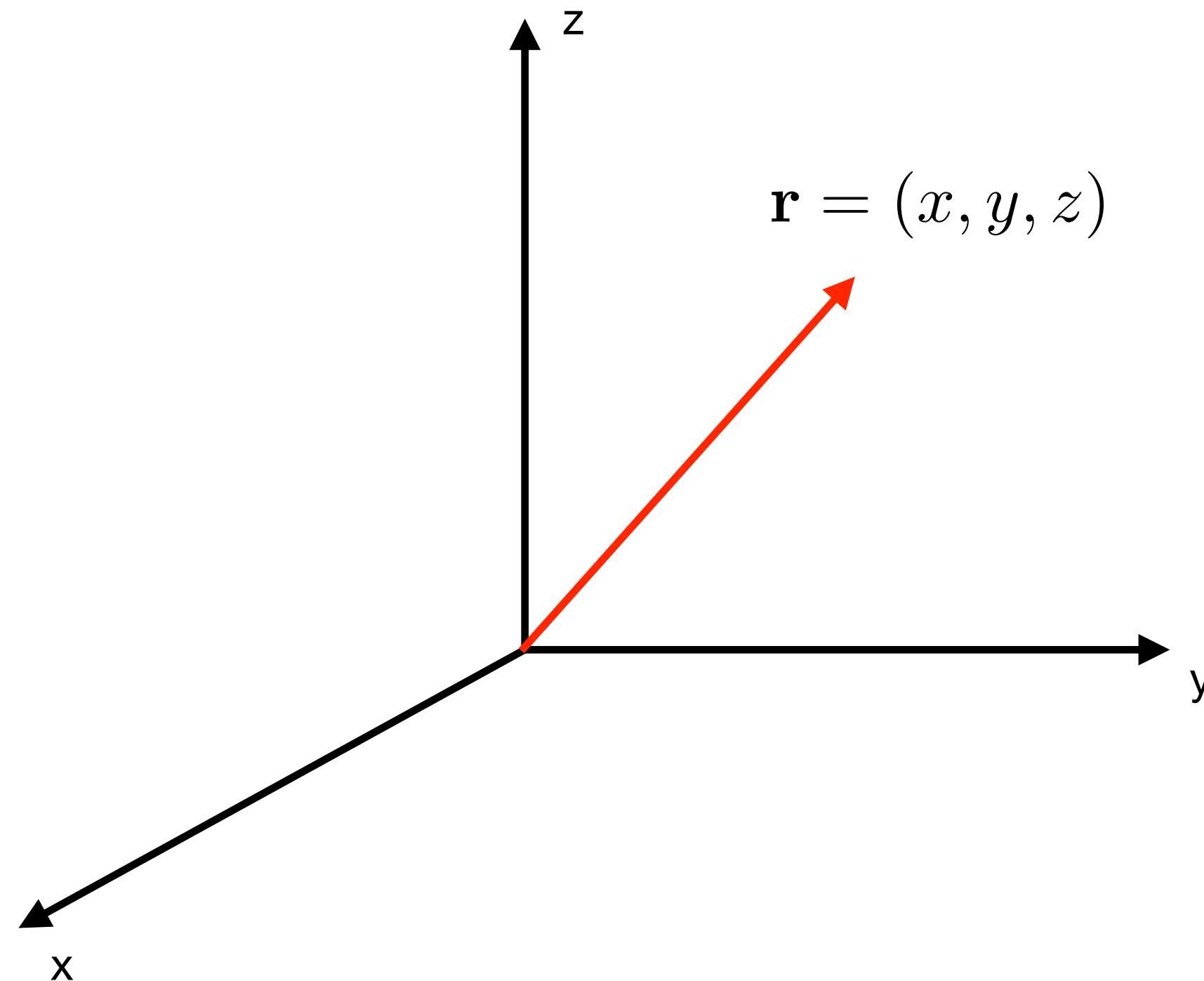
This is called a **Born-Oppenheimer Approximation**. Since this system has spherical symmetry, we should use Laplacian operator in spherical coordinates representation.

$$\hat{H} = -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] - \frac{e^2}{4\pi\epsilon_0 r}$$

Math: Spherical Coordinates

How can we represent a point in \mathbb{R}^3 ? The most familiar way is *Cartesian coordinates*.

In **spherical coordinates**, a point is represented by one distance and two angles.



First variable is r , distance from the origin.

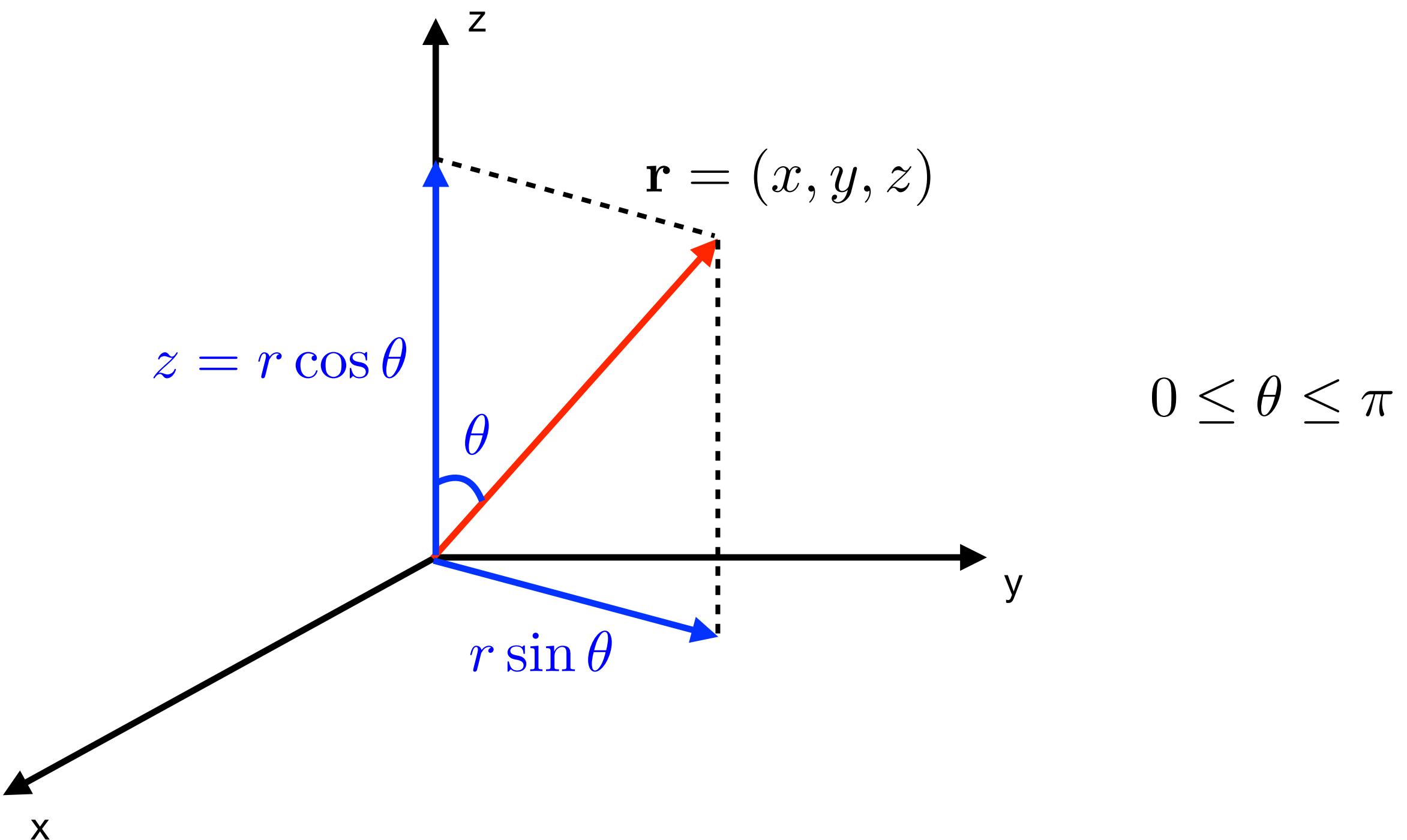
$$r = \sqrt{x^2 + y^2 + z^2}$$

Therefore, range of r is

$$0 \leq r < \infty$$

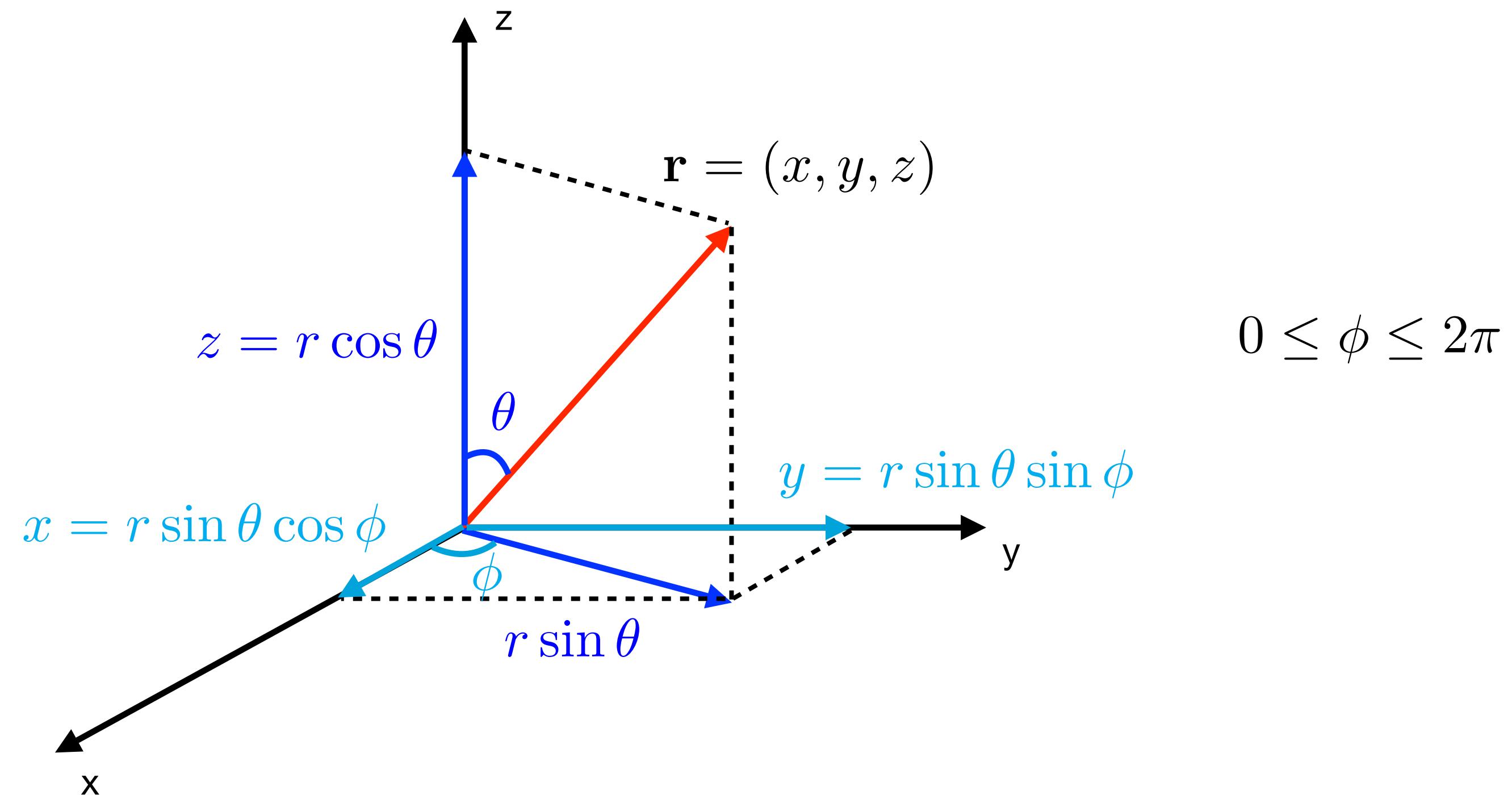
Math: Spherical Coordinates

Second variable is *polar angle*, angle with respect to z axis.



Math: Spherical Coordinates

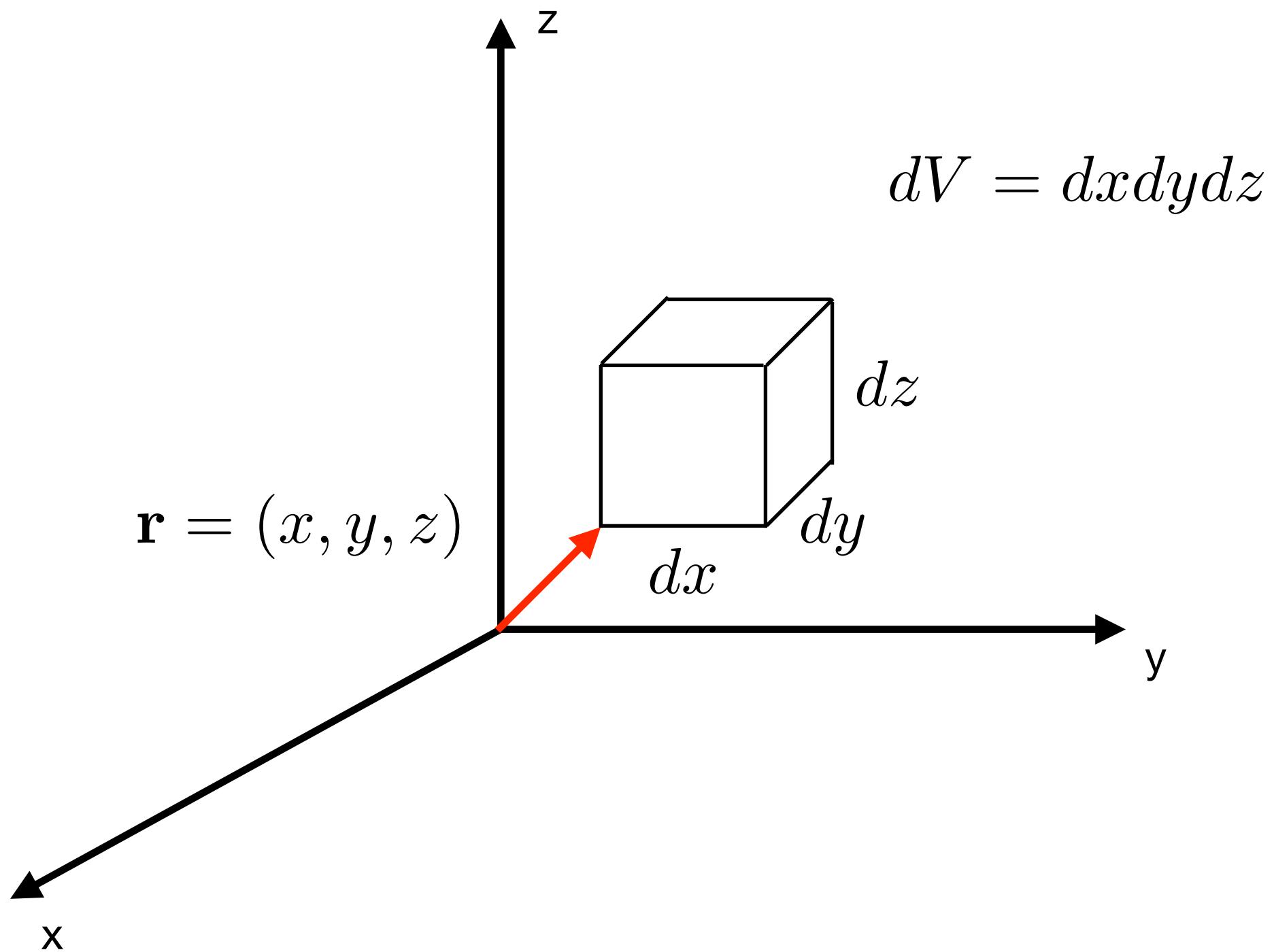
Third variable is *azimuthal angle*, angle of rotation from the x axis.



Math: Spherical Coordinates

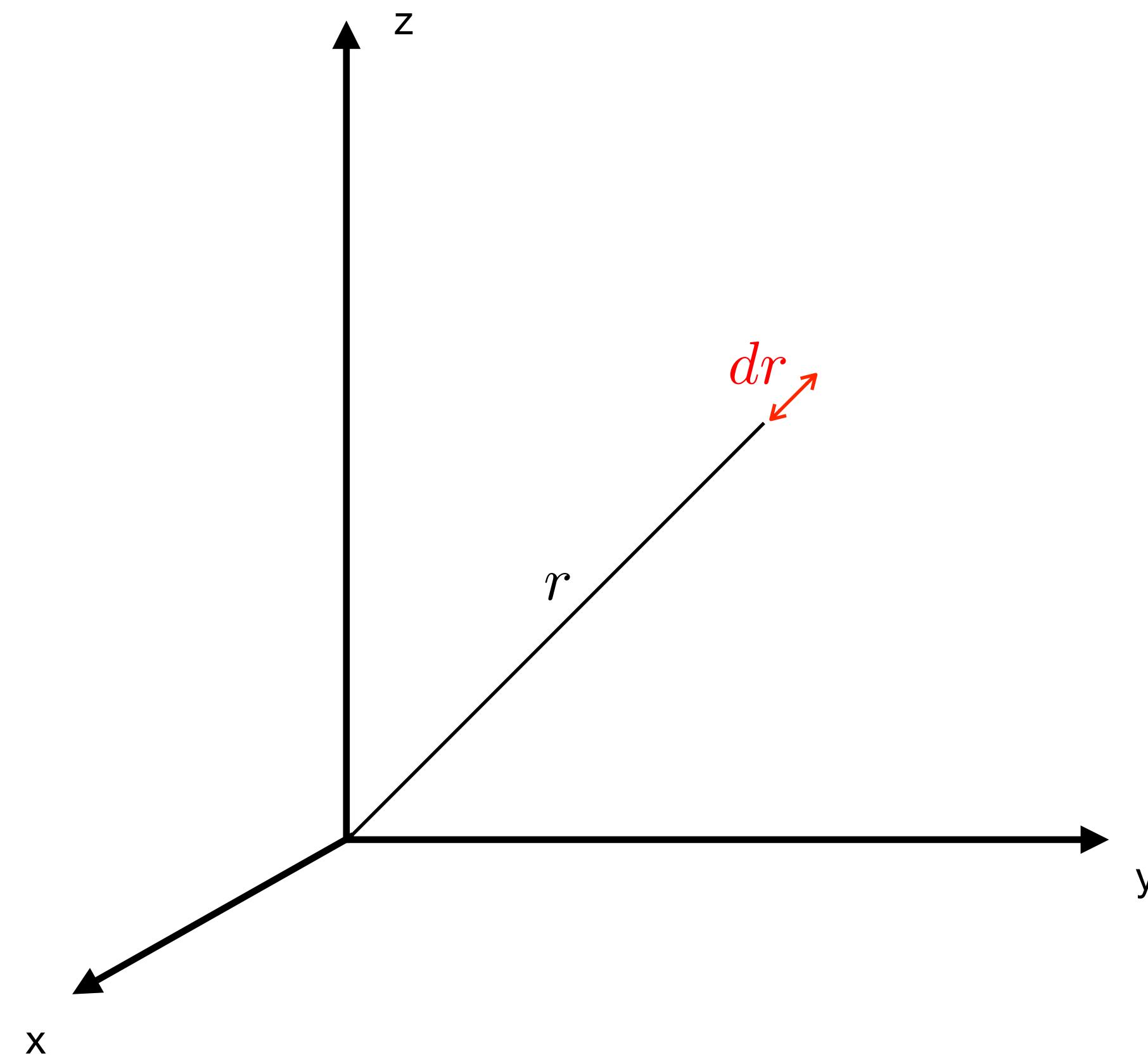
Let's consider the area and volume element in spherical coordinates. We need this for integration.

Remind the Cartesian case.



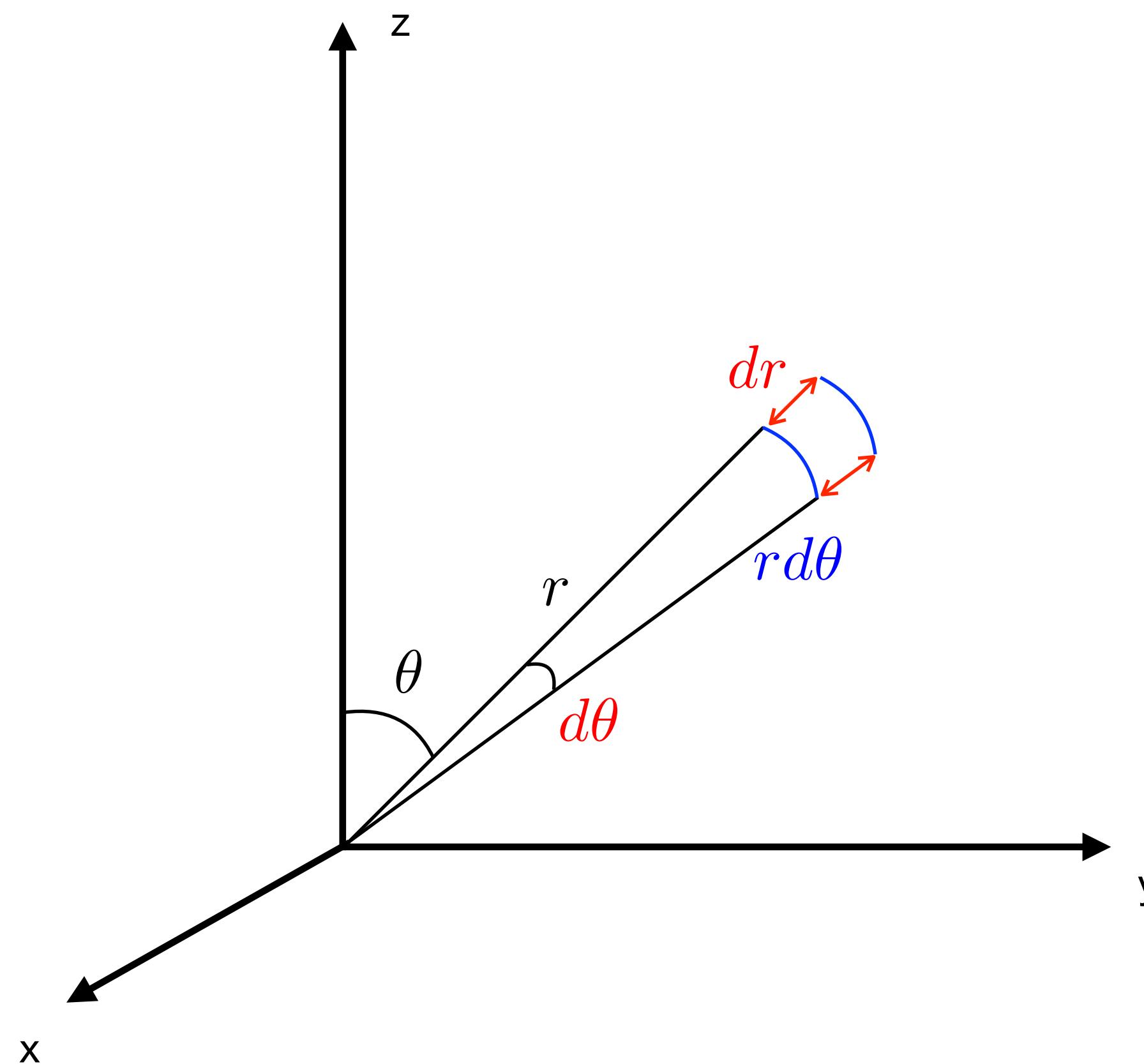
Math: Spherical Coordinates

Similar in spherical case. Go a little bit in r, θ, ϕ direction and calculate the infinitesimal volume.



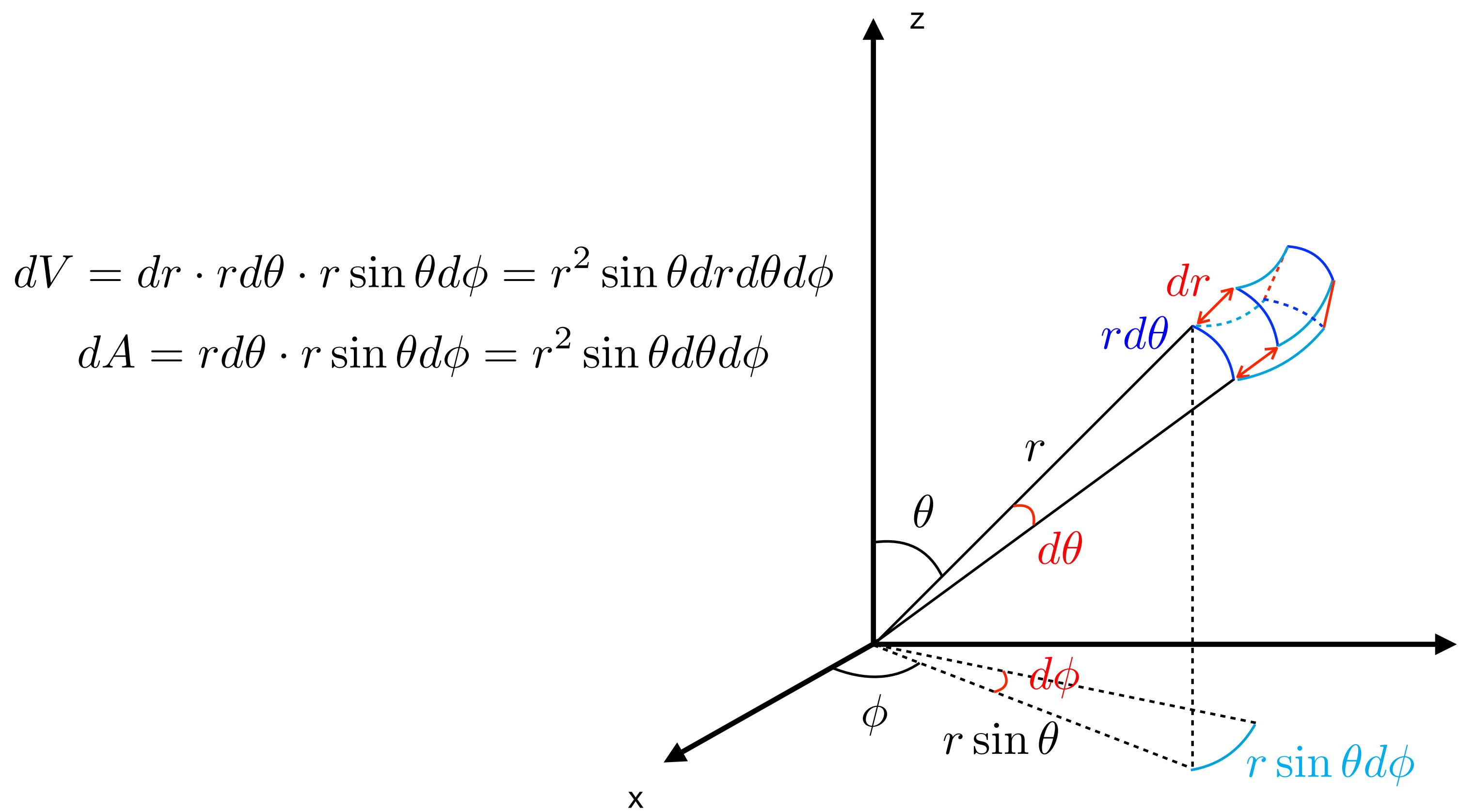
Math: Spherical Coordinates

Similar in spherical case. Go a little bit in r, θ, ϕ direction and calculate the infinitesimal volume.



Math: Spherical Coordinates

Similar in spherical case. Go a little bit in r, θ, ϕ direction and calculate the infinitesimal volume.



Math: Spherical Coordinates

Let's do some exercise.

Q1. Calculate the volume of a sphere with radius R .

$$V = \int dV = \int_0^R \int_0^\pi \int_0^{2\pi} r^2 \sin \theta dr d\theta d\phi = \int_0^\infty r^2 dr \cdot \int_0^\pi \sin \theta d\theta \cdot \int_0^{2\pi} d\phi = \frac{R^3}{3} \cdot 2 \cdot 2\pi = \frac{4}{3}\pi R^3$$

Q2. Calculate the surface area of a sphere with radius R .

$$A = \int dA = \int_0^\pi \int_0^{2\pi} R^2 \sin \theta d\theta d\phi = R^2 \cdot \int_0^\pi \sin \theta d\theta \cdot \int_0^{2\pi} d\phi = R^2 \cdot 2 \cdot 2\pi = 4\pi R^2$$

Math: Spherical Coordinates Glossaries

When it comes to infinitesimal volume, sometimes we want coordinate-neutral form.

$$d\tau$$

In case of spherical coordinates, part of volume element including angular part is called a **solid angle**.

$$r^2 dr \cdot \sin \theta d\theta d\phi \equiv r^2 dr d\Omega$$

Solid angle of a sphere is

$$\int d\Omega = \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi = 4\pi$$

Separation of variables

Hamiltonian of hydrogen atom is

$$\hat{H} = -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] - \frac{e^2}{4\pi\epsilon_0 r}$$

Schrödinger equation:

$$\hat{H}\psi(r, \theta, \phi) = E\psi(r, \theta, \phi)$$

Separation of variables: Assume that wavefunction can be separated into two independent functions.

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$$

Separation of variables

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] - \frac{e^2}{4\pi\epsilon_0 r} \psi = E\psi$$

Multiply $2mr^2$ both side.

$$-\hbar^2 \left[\frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] - 2mr^2 \left[\frac{e^2}{4\pi\epsilon_0 r} + E \right] \psi = 0$$

Substitute $\psi = RY$.

$$-\hbar^2 \left[Y \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{R}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{R}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right] - 2mr^2 \left[\frac{e^2}{4\pi\epsilon_0 r} + E \right] RY = 0$$

Separation of variables

Divide with RY.

$$-\frac{\hbar^2}{R(r)} \left[\frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2mr^2}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) R(r) \right] - \frac{\hbar^2}{Y(\theta, \phi)} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right] = 0$$

Then, first and second terms are independent of each other (they depend on different kind of variables).

Therefore, two terms should be identical as *constants*.

$$-\frac{1}{R(r)} \left[\frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2mr^2}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) R(r) \right] = -l(l+1)$$

$$-\frac{1}{Y(\theta, \phi)} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right] = l(l+1)$$

Separation of variables

Fortunately, the second equation is a well-known one.

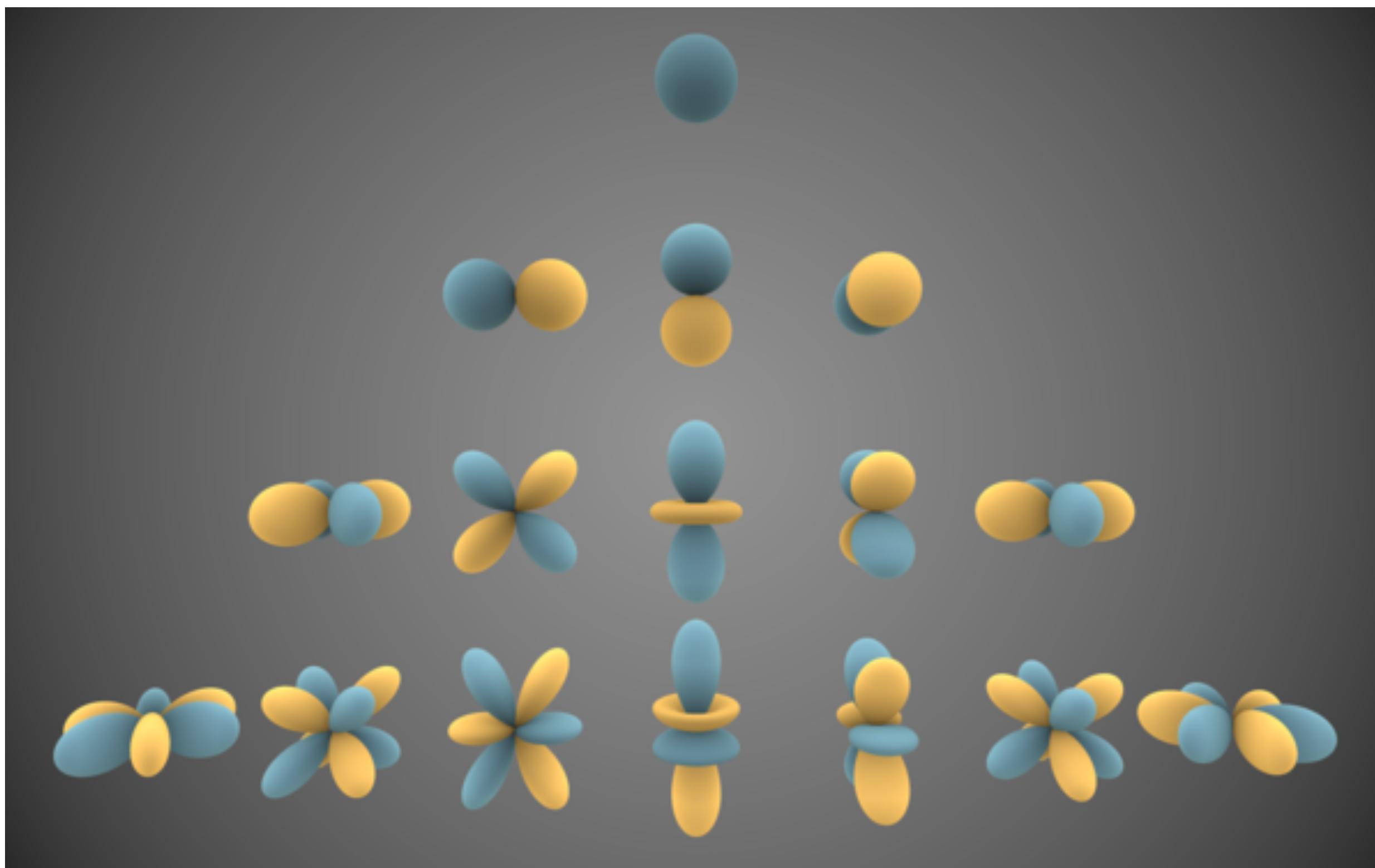
$$-\frac{1}{Y(\theta, \phi)} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right] = l(l+1)$$

Solution of this equation is called **spherical harmonics**.

$$Y_l^m(\theta, \phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos \theta) e^{im\phi}$$

Where $P_l^m(\cos \theta)$ denotes *associated Legendre polynomials*, which are solutions of another well-known differential equation.

Spherical Harmonics



Hydrogen atom wavefunction

The remaining equation can be solved by existing methods, but we won't solve it here.

$$-\frac{1}{R(r)} \left[\frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2mr^2}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) R(r) \right] = -l(l+1)$$

By solving radial equation, we can obtain (1) energy eigenvalues, (2) relation between n and l , (3) total wavefunction, where L denotes associated *Laguerre polynomial*, another special function.

$$R_{nl}(r) = -\sqrt{\frac{(n-l-1)!}{2n[(n+1)!]^3}} \left(\frac{2}{na_0} \right)^{l+3/2} r^l e^{-r/na_0} L_{n+l}^{2l+1} \left(\frac{2r}{na_0} \right)$$

$$E_n = -\frac{e^2}{8\pi\epsilon_0 a_0 n^2} \quad n = 1, 2, 3, \dots$$

Hydrogen atom wavefunction

TABLE 6.5

The complete hydrogenlike atomic wave functions for $n = 1$, 2, and 3. The quantity Z is the atomic number of the nucleus, and $\sigma = Zr/a_0$, where a_0 is the Bohr radius.

$n = 1,$	$l = 0,$	$m = 0$	$\psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma}$
$n = 2,$	$l = 0,$	$m = 0$	$\psi_{200} = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0}\right)^{3/2} (2 - \sigma) e^{-\sigma/2}$
	$l = 1,$	$m = 0$	$\psi_{210} = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2} \cos \theta$
	$l = 1,$	$m = \pm 1$	$\psi_{21\pm 1} = \frac{1}{\sqrt{64\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2} \sin \theta e^{\pm i\phi}$
$n = 3,$	$l = 0,$	$m = 0$	$\psi_{300} = \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0}\right)^{3/2} (27 - 18\sigma + 2\sigma^2) e^{-\sigma/3}$
	$l = 1,$	$m = 0$	$\psi_{310} = \frac{1}{81} \left(\frac{2}{\pi}\right)^{1/2} \left(\frac{Z}{a_0}\right)^{3/2} (6\sigma - \sigma^2) e^{-\sigma/3} \cos \theta$
	$l = 1,$	$m = \pm 1$	$\psi_{31\pm 1} = \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} (6\sigma - \sigma^2) e^{-\sigma/3} \sin \theta e^{\pm i\phi}$
	$l = 2,$	$m = 0$	$\psi_{320} = \frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3} (3 \cos^2 \theta - 1)$
	$l = 2,$	$m = \pm 1$	$\psi_{32\pm 1} = \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta e^{\pm i\phi}$
	$l = 2,$	$m = \pm 2$	$\psi_{32\pm 2} = \frac{1}{162\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta e^{\pm 2i\phi}$

s orbitals

$$\psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-\sigma}$$

$$\psi_{200} = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (2 - \sigma) e^{-\sigma/2}$$

$$\psi_{300} = \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (27 - 18\sigma + 2\sigma^2) e^{-\sigma/3}$$

$$\sigma = \frac{Zr}{a_0}$$

If $l=0$, orbitals are called s orbitals. These orbitals contain no angular part: therefore, spherically symmetric.

s orbitals

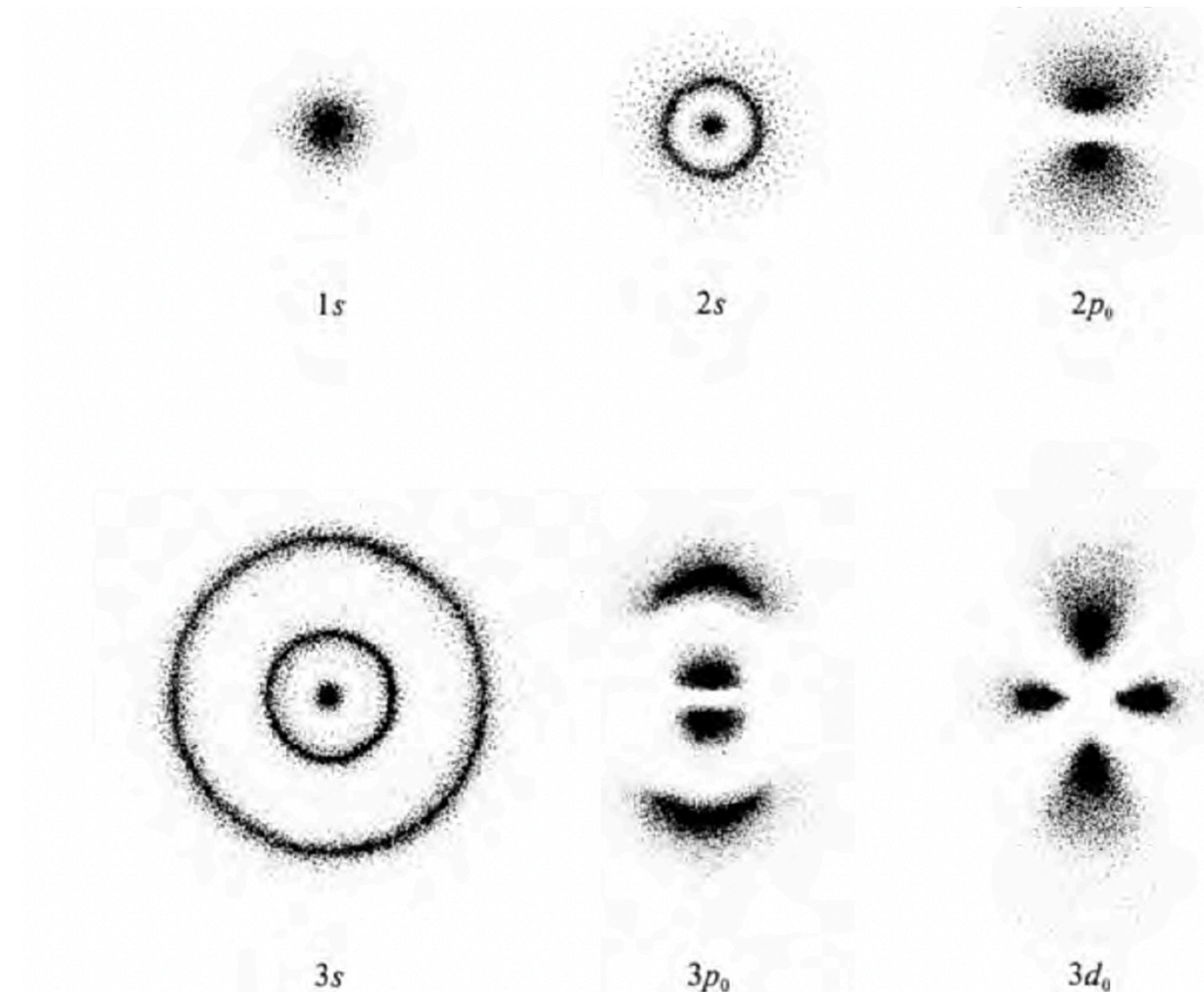


FIGURE 6.5

Probability density plots of some hydrogen atomic orbitals. The density of the dots is proportional to the probability of finding the electron in that region.

p orbitals

$$\begin{array}{llll} n = 2, & l = 0, & m = 0 & \psi_{200} = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0}\right)^{3/2} (2 - \sigma) e^{-\sigma/2} \quad 2s \\ & & & \\ l = 1, & m = 0 & \psi_{210} = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2} \cos \theta \quad 2p_z \\ & & & \\ l = 1, & m = \pm 1 & \psi_{21\pm 1} = \frac{1}{\sqrt{64\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2} \sin \theta e^{\pm i\phi} & ? \end{array}$$

Take appropriate **linear combination** to obtain “real” wavefunction.

The p_x , p_y orbitals we know is constructed via linear combination.

$$\begin{aligned} p_x &= \frac{1}{\sqrt{2}} (Y_1^1 + Y_1^{-1}) \\ p_y &= \frac{1}{\sqrt{2}i} (Y_1^1 - Y_1^{-1}) \end{aligned}$$

Mathematical form of orbitals is not unique and we can choose certain form.

p orbitals

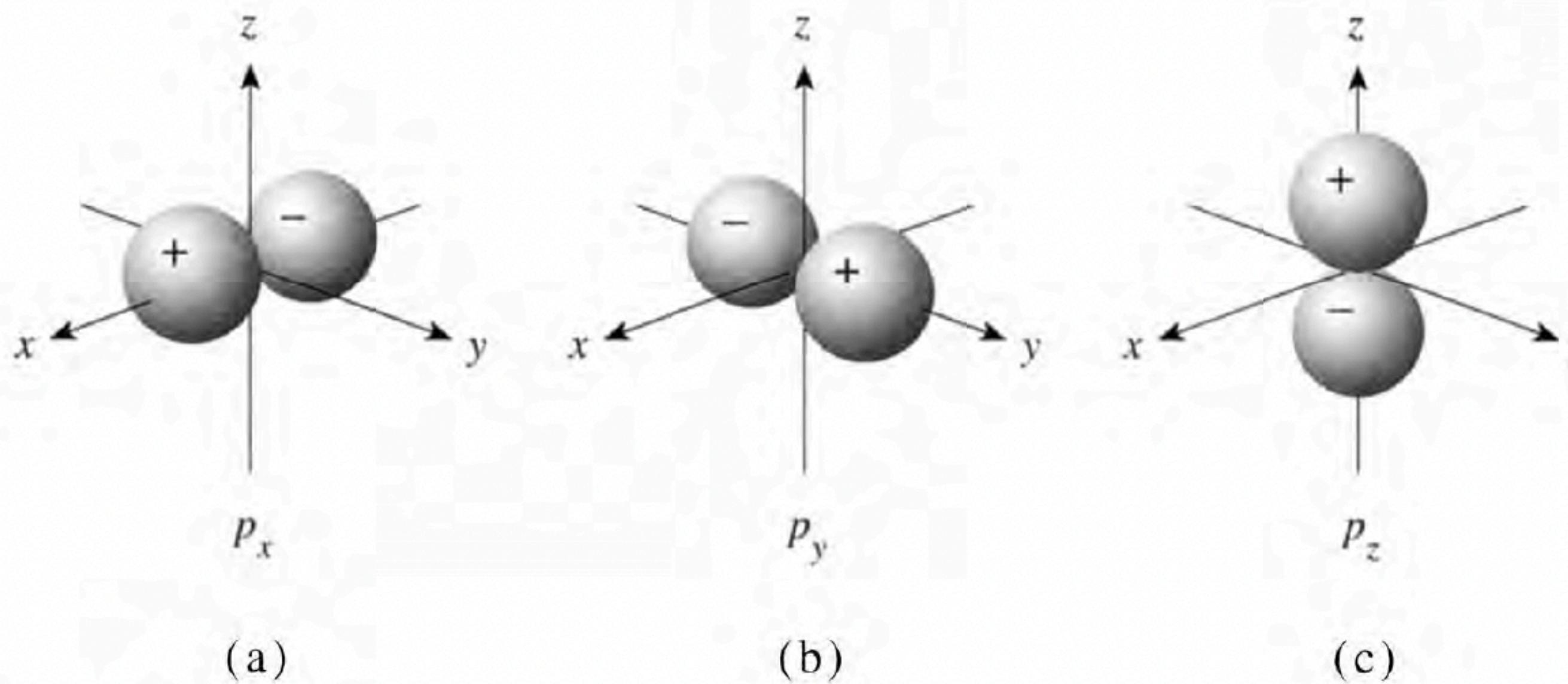


FIGURE 6.4

Three-dimensional polar plots of the angular part of the real representation of the hydrogen atomic wave functions for $l = 1$ (see Equations 6.62 for real representations of p_x and p_y .)

Interlude

Therefore we obtained **AO** (atomic orbital) of hydrogen.

Orbital is defined as a single-electron wavefunction.

How can we calculate the orbitals of multielectron atoms?

Helium atom

The Hamiltonian under Born-Oppenheimer approximation is

$$\hat{H} = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{2e^2}{4\pi\epsilon_0} \left(\frac{1}{r_1} + \frac{1}{r_2} \right) + \frac{e^2}{4\pi\epsilon_0 r_{12}}$$

Due to the *electron-electron repulsion*, multielectron atoms cannot be solved exactly.

Therefore Schrödinger equation should be solved *approximately*, or *numerically*.

In **atomic unit** ($\hbar = m_e = e = 4\pi\epsilon_0 = 1$),

$$\hat{H} = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}$$

Hartree-Fock approximation

The simplest approximation we can consider is - representing the wavefunction as a product of two single-electron wavefunctions (product of hydrogen atomic orbitals).

$$\psi(\mathbf{r}_1, \mathbf{r}_2) \simeq \phi(\mathbf{r}_1)\phi(\mathbf{r}_2)$$

This is **Hartree-Fock approximation**.

Hartree-Fock approximation

Classically, probability density of electron can be interpreted as a charge density. Therefore, electric potential energy experienced by electron 1 (which is generated by electron 2) is

$$V_1^{\text{eff}}(\mathbf{r}_1) = \int \phi^*(\mathbf{r}_2) \frac{1}{r_{12}} \phi(\mathbf{r}_2) d\mathbf{r}_2$$

Then, “effective” Hamiltonian for electron 1 is

$$\hat{H}_1 = -\frac{1}{2} \nabla_1^2 - \frac{2}{r_1} + V_1^{\text{eff}}(\mathbf{r}_1)$$

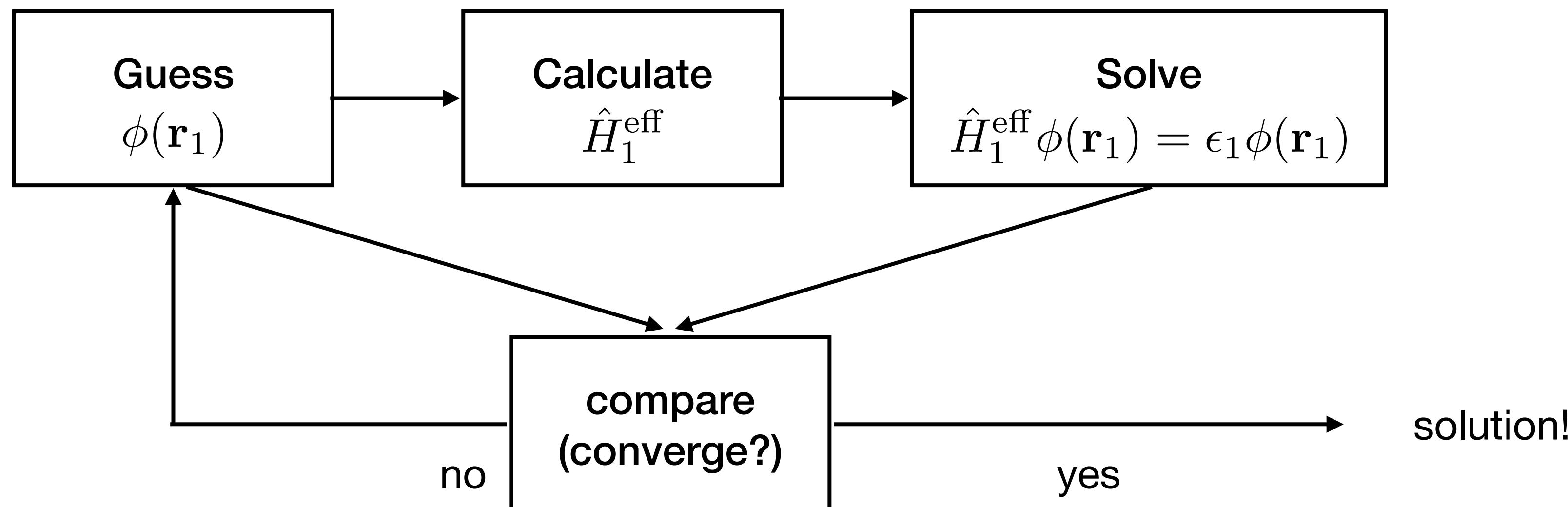
The Schrödinger equation corresponding to this Hamiltonian is

$$\hat{H}_1 \phi(\mathbf{r}_1) = \epsilon_1 \phi(\mathbf{r}_1)$$

Hartree-Fock approximation

Note that the form of $\phi(\mathbf{r}_1)$ and $\phi(\mathbf{r}_2)$ are essentially same (two electrons are indistinguishable). So to speak, we should know the solution $\phi(\mathbf{r}_2)$ in order to get solution $\phi(\mathbf{r}_1)$.

The method of solving an equation like this is by a scheme called the **self-consistent field (SCF) method**.



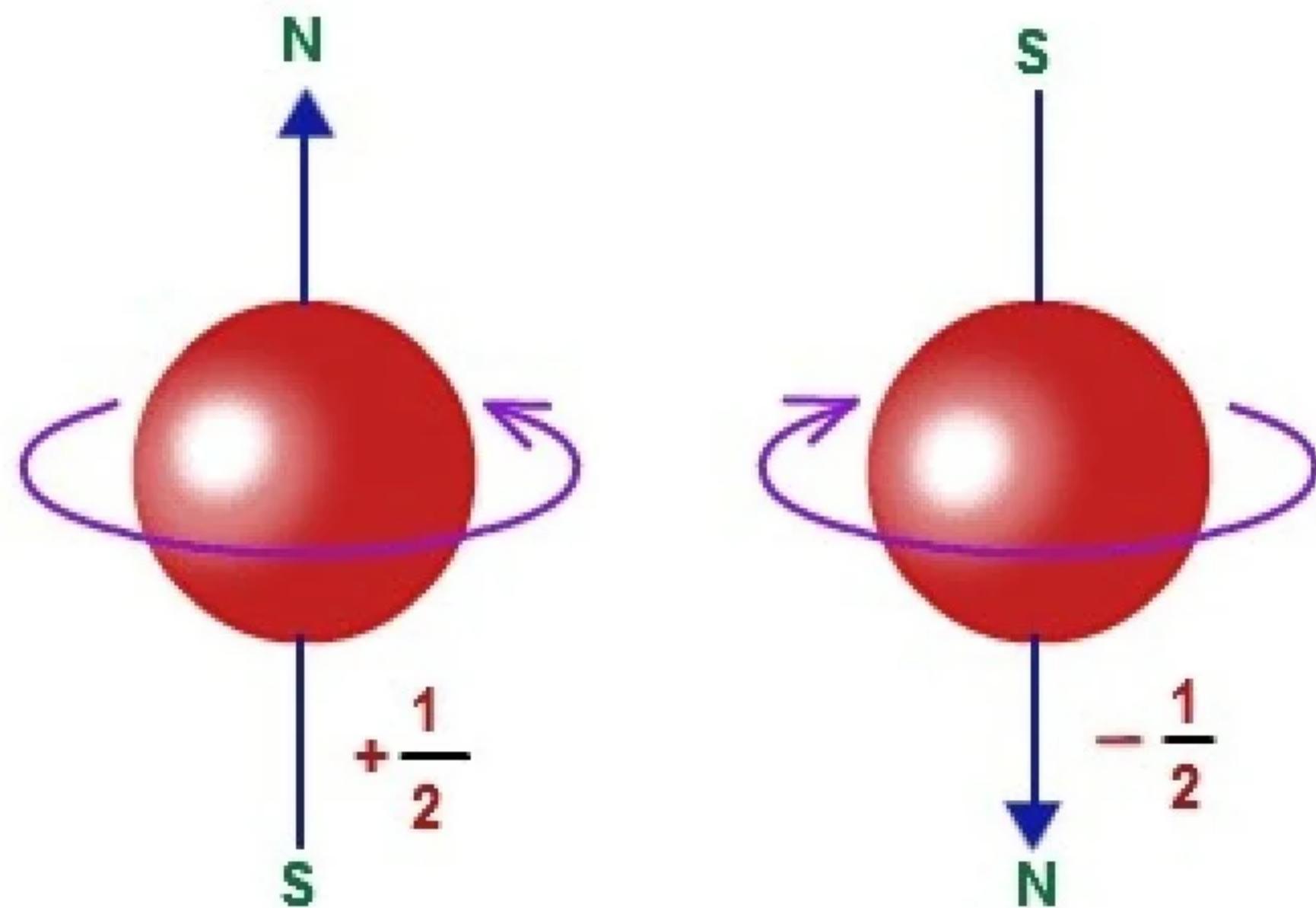
Electron spin

For He atom, two electrons occupies 1s orbital, which is identical.

However, for Li atom, we cannot put three electrons in 1s orbital, due to the **Pauli exclusion principle**.

Actually there is more serious problem: **the electron spin**.

Electron spin explained: imagine a ball that's rotating, except it's not a ball and it's not rotating

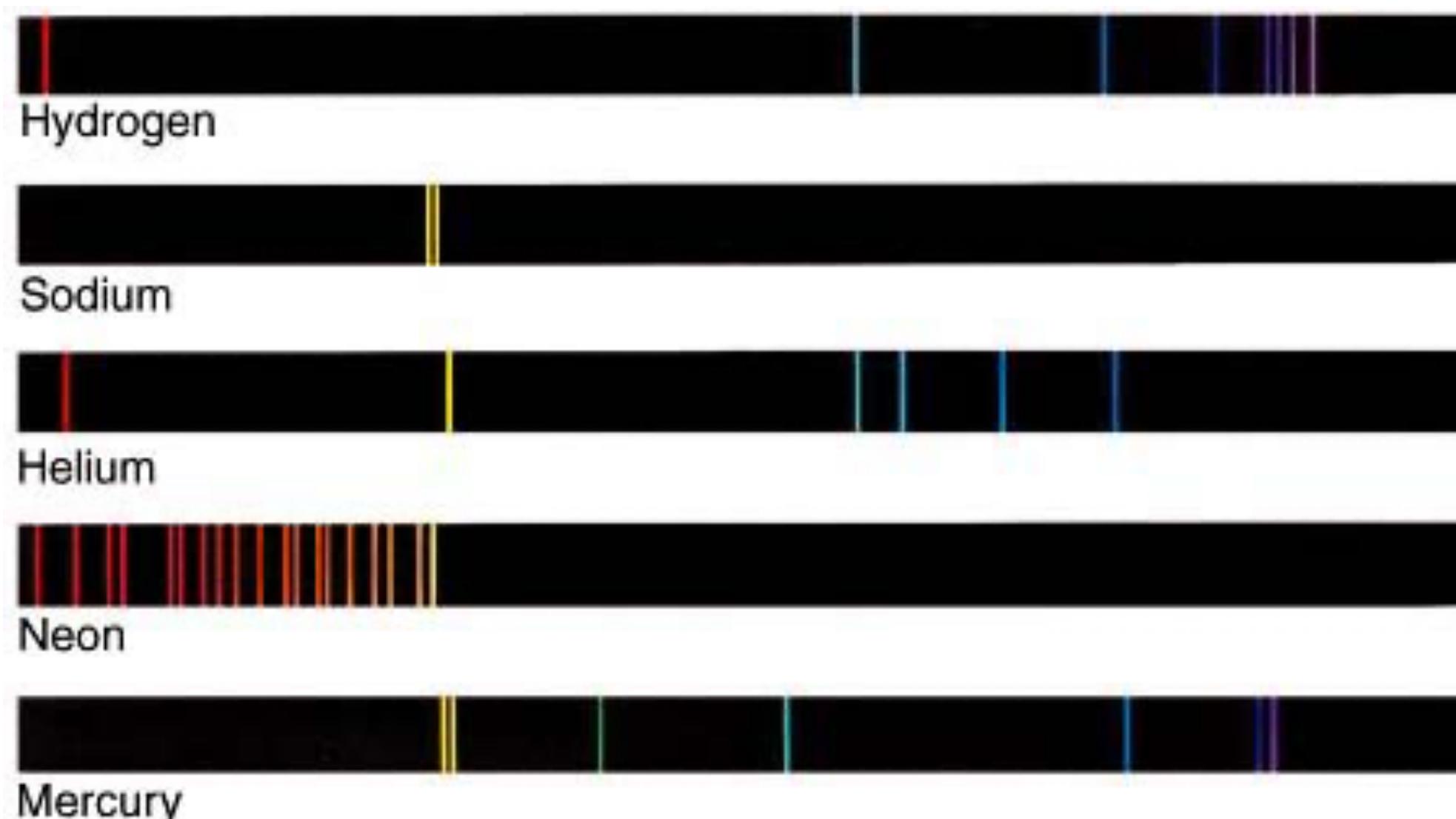


Electron spin

The Schrödinger equation predicts emission spectrum at ~ 590 nm, which is yellow color.

However two closely spaced lines (a doublet) are observed at 589.59 nm and 588.99 nm.

This is due to the fourth quantum number, **spin quantum number**.



Electron spin

An electron can have up spin, α or down spin β . It can be measured via spin operator.

$$\hat{S}_z |\alpha\rangle = \frac{\hbar}{2} |\alpha\rangle, \quad \hat{S}_z |\beta\rangle = -\frac{\hbar}{2} |\beta\rangle$$

Pauli exclusion principle: No two electrons in an atom can have the same values of all four quantum numbers. I assume that we already know this version of exclusion principle.

Pauli exclusion principle - advanced version:

Wavefunction is **antisymmetric** under the interchange of two electrons.

$$\Psi(1, 2) = -\Psi(2, 1)$$

Antisymmetric wavefunction

Note that two electrons are *indistinguishable*. So (electron 1 in orbital 1 + electron 2 in orbital 2) is equivalent to (electron 1 in orbital 2 + electron 2 in orbital 1).

Mathematically, indistinguishability requires that we should take linear combinations involving all possible labelings of the electrons. In case of ground state He atom,

$$\begin{aligned}\Psi_s &= \psi(1, 2) + \psi(2, 1) = 1s\alpha(1)1s\beta(2) + 1s\alpha(2)1s\beta(1) \\ \Psi_a &= \psi(1, 2) - \psi(2, 1) = 1s\alpha(1)1s\beta(2) - 1s\alpha(2)1s\beta(1)\end{aligned}$$

The second one is antisymmetric under the labeling change, therefore it is acceptable.

Antisymmetric wavefunction

Consider a situation putting two electrons into three $2p$ orbitals. Let's separate into spin and spatial part.

$\alpha(1)\alpha(2)$: symmetric

$\beta(1)\beta(2)$: symmetric

$\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)]$: symmetric

$\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)]$: antisymmetric

possible spin configurations

$\phi_{2p_x}(1)\phi_{2p_x}(2)$: symmetric

$\frac{1}{\sqrt{2}}[\phi_{2p_x}(1)\phi_{2p_y}(2) + \phi_{2p_y}(1)\phi_{2p_x}(2)]$: symmetric

$\frac{1}{\sqrt{2}}[\phi_{2p_x}(1)\phi_{2p_y}(2) - \phi_{2p_y}(1)\phi_{2p_x}(2)]$: antisymmetric

possible spatial configurations

Antisymmetric wavefunction

If two electrons occupy the same spatial orbital, spatial part is symmetric. Therefore, due to the Pauli exclusion, spin part should be antisymmetric: opposite spins! This state is called a **singlet** state.

$\alpha(1)\alpha(2)$: symmetric

$\beta(1)\beta(2)$: symmetric

$\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)]$: symmetric

$\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)]$: antisymmetric

possible spin configurations

$\phi_{2p_x}(1)\phi_{2p_x}(2)$: symmetric

$\frac{1}{\sqrt{2}}[\phi_{2p_x}(1)\phi_{2p_y}(2) + \phi_{2p_y}(1)\phi_{2p_x}(2)]$: symmetric

$\frac{1}{\sqrt{2}}[\phi_{2p_x}(1)\phi_{2p_y}(2) - \phi_{2p_y}(1)\phi_{2p_x}(2)]$: antisymmetric

possible spatial configurations

Antisymmetric wavefunction

If two electrons occupy different orbitals, two cases arise. Symmetric spatial configuration matches antisymmetric spin configuration.

$\alpha(1)\alpha(2)$: symmetric

$\beta(1)\beta(2)$: symmetric

$\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)]$: symmetric

$\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)]$: antisymmetric

possible spin configurations

$\phi_{2p_x}(1)\phi_{2p_x}(2)$: symmetric

$\frac{1}{\sqrt{2}}[\phi_{2p_x}(1)\phi_{2p_y}(2) + \phi_{2p_y}(1)\phi_{2p_x}(2)]$: symmetric

$\frac{1}{\sqrt{2}}[\phi_{2p_x}(1)\phi_{2p_y}(2) - \phi_{2p_y}(1)\phi_{2p_x}(2)]$: antisymmetric

possible spatial configurations

Antisymmetric wavefunction

Antisymmetric spatial configuration matches with symmetric spin configuration - three states arise. These states are called **triplet**.

$\alpha(1)\alpha(2)$: symmetric

$\beta(1)\beta(2)$: symmetric

$\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)]$: symmetric

$\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)]$: antisymmetric

$\phi_{2p_x}(1)\phi_{2p_x}(2)$: symmetric

$\frac{1}{\sqrt{2}}[\phi_{2p_x}(1)\phi_{2p_y}(2) + \phi_{2p_y}(1)\phi_{2p_x}(2)]$: symmetric

$\frac{1}{\sqrt{2}}[\phi_{2p_x}(1)\phi_{2p_y}(2) - \phi_{2p_y}(1)\phi_{2p_x}(2)]$: antisymmetric

possible spin configurations

possible spatial configurations

Antisymmetric wavefunction

Antisymmetry of electronic wavefunction can be encoded easily by utilizing **determinant**. This form is called the **Slater determinant**.

$$\Psi(1, 2, \dots, N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_1(1) & u_2(1) & \cdots & u_N(1) \\ u_1(2) & u_2(2) & \cdots & u_N(2) \\ \vdots & \vdots & \ddots & \vdots \\ u_1(N) & u_2(N) & \cdots & u_N(N) \end{vmatrix} \quad (8.44)$$

$$\Psi = \frac{1}{\sqrt{3!}} \begin{vmatrix} 1s\alpha(1) & 1s\beta(1) & 2s\alpha(1) \\ 1s\alpha(2) & 1s\beta(2) & 2s\alpha(2) \\ 1s\alpha(3) & 1s\beta(3) & 2s\alpha(3) \end{vmatrix}$$

References of this lecture

If you are interested in obtaining full solution of hydrogen atom,

Check for the additional note I will upload in GitHub.

If you are interested in the details about today's lecture,

McQuarrie, D. A.; Simon, J. D. *Physical Chemistry: A Molecular Approach*, 2nd ed.; University Science Books, 1997.

Atkins' Physical Chemistry textbook is always your companion, even though I do not mention it.