

Applications to atomic systems

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Recapitulate

- We have shown how quantum mechanics can be used to explain particle motion in 1-D.
- The instantaneous state of a particle is fully specified by a complex wavefunction $\psi(x, t)$.
- The probability of finding the particle at a time t between x and $x + dx$ is

$$P(x, t)dx = |\psi(x, t)|^2 dx \text{ where } \int_{-\infty}^{\infty} |\psi(x, t)|^2 dx = 1 \text{ at all times.}$$

- Two new features have emerged from the study of 1-D systems:
1. Quantization of Energy 2. Tunneling Phenomena

We now extend to 3-D systems and explore the predictions of the theory for —
Particle in a box, 3D Oscillator and Hydrogen atom

Learning objectives

By the end of this part, you will be able to:

- 1 Describe quantum mechanics in higher dimensions.
- 2 Understand the concept of degeneracy.
- 3 Applications of model 3-D systems to “real world”.

Quantum mechanics in 3-D

Fundamental concepts in 3-D: Extensions from 1-D

- Generalize $p_x \longrightarrow \frac{\hbar}{i} \frac{\partial}{\partial x}$ to 3-D. Cartesian coordinates have no preferential directions

$$p_x \longrightarrow \frac{\hbar}{i} \frac{\partial}{\partial x}, p_y \longrightarrow \frac{\hbar}{i} \frac{\partial}{\partial y}, p_z \longrightarrow \frac{\hbar}{i} \frac{\partial}{\partial z} \quad \mathbf{p} \longrightarrow \frac{\hbar}{i} \nabla$$

- In 3-D, the instantaneous state of a particle is fully specified by $\psi(\mathbf{x}, \mathbf{y}, \mathbf{z}, t)$.
- By analogy with 1-D systems, the probability to find the particle at time t between x and $x + dx$, between y and $y + dy$, and between z and $z + dz$, is

$$P(x, y, z, t) dx dy dz = |\psi(x, y, z, t)|^2 dx dy dz \quad (1)$$

- Like in 1-D, this interpretation of the wavefunction only makes sense if the wavefunction is normalized:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\psi(x, y, z, t)|^2 dx dy dz = 1 \quad (2)$$

- In 3-D, the time-dependent Schroedinger equation is:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(x, y, z) \psi \quad \text{where} \quad \nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (3)$$

Fundamental concepts in 3-D: Differences from 1-D

- In 1-D, knowing x uniquely determined $\psi(x)$.
In 3-D, knowing the three quantities x , y , and z can only define the state $\psi(x, y, z)$.
- **1-D bound states:** Integer energy level n contains all the information about the particle.
- **3-D bound states:** Three quantum numbers are needed to specify the condition. These correspond to the three independent degrees of freedom for a particle in space:

$$\text{1-D: } \{E_n, \psi_n(x)\} \quad \text{3-D: } \{E_{n,m,l}, \psi_{n,m,l}(x, y, z)\}$$

- Unlike in 1-D, we can have situation where different states have the same energy!

$$E_{n_1, m_1, l_1} = E_{n_2, m_2, l_2} \quad \psi_{n_1, m_1, l_1} \neq \psi_{n_2, m_2, l_2} \quad \text{This is referred to as degeneracy}$$

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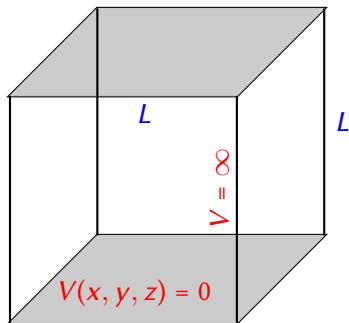
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Two or more stationary states of the same quantum-mechanical system may have the same energy even though their wave functions are not the same.

Particle in 3-D box

Particle in 3-D box



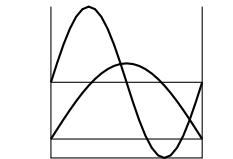
- Consider 3-D version of particle in a box with all sides L .
- Like in 1-D, $\psi(x, y, z)$ must be zero at the walls of the box.
- Following 1-D, we can try the following solution:

$$\psi(x, y, z) = \phi(x) \eta(y) \zeta(z)$$

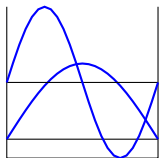
- Inserting this in time-independent Schroedinger equation:

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi = E\psi$$

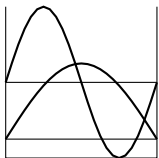
Particle in 3-D box



$x = 0$ $x = L$



$y = 0$ $y = L$



$z = 0$ $z = L$

- We have 3 identical equations to solve in three dimensions:

$$-\frac{\hbar^2}{2m} \frac{d^2 \phi(x)}{dx^2} = E_x \phi(x)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \eta(y)}{dy^2} = E_y \eta(y)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \zeta(z)}{dz^2} = E_z \zeta(z)$$

The solution is

$$\psi_{n_x, n_y, n_z}(x, y, z) = \phi_{n_x}(x) \eta_{n_y}(y) \zeta_{n_z}(z) = A \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

- Applying boundary conditions, we get

$$E = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2); \quad k_x = \frac{\pi n_x}{L}, \quad k_y = \frac{\pi n_y}{L}, \quad k_z = \frac{\pi n_z}{L}$$

Particle in 3-D box

n_x	n_y	n_z	n^2	Degeneracy
1	1	1	3	None
1	1	2	6	
1	2	1	6	
2	1	1	6	Threefold
1	2	2	9	
2	1	2	9	
2	2	1	9	Threefold
1	1	3	11	
1	3	1	11	
3	1	1	11	None
2	2	2	12	

- Energy eigenvalues are

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2) \quad n_x, n_y, n_z \in 1, 2, \dots, \quad (4)$$

- Wavefunctions are

$$\psi_{n_x, n_y, n_z} = A \sin\left(\frac{\pi n_x}{L} x\right) \sin\left(\frac{\pi n_y}{L} y\right) \sin\left(\frac{\pi n_z}{L} z\right) \quad (5)$$

- Ground state is $n_x = n_y = n_z = 1$
- First excited state can be obtained in 3 different ways:

$$n_x = n_y = 1, n_z = 2; \quad n_z = n_x = 1, n_y = 2; \quad n_x = 2, n_y = n_z = 1$$

Corresponding ψ 's are different \Rightarrow Degenerate states

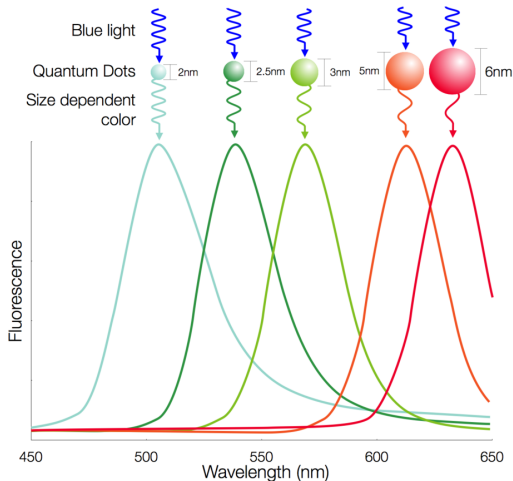
“Real world” Particle in 3-D box

Quantum Dots

- A quantum dot is a very small structure, e.g. a semiconductor nanocrystal embedded in another semiconductor material, which can confine electrons or other carriers in all three dimensions.
- The confinement of electron in all three dimensions is like particle in 3-D box!
- Like particle (atom) in a box, an ideal isolated quantum dot has discrete energy levels.
- Quantum dots can be considered as artificial atoms where the energy levels can be adjusted by design, e.g. by controlling the quantum dot dimensions or the material composition
- If the size of the quantum dot is small enough that the quantum confinement effects dominate (typically less than 10 nm), the electronic and optical properties are highly tunable.

Quantum Dots

Quantum Dot Size and Color



Next generation display (TV) screens will use Quantum dots technology.

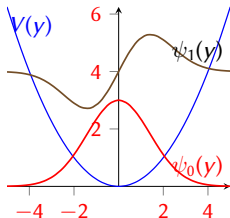
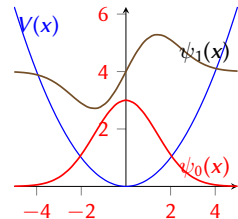
Several advantages:

- 1 The color of light each quantum dot gives is **very stable and pure**.
- 2 Quantum dots can show **precise colors** while the light from LEDs get mixed with adjacent colors.
- 3 The 3 primary colors are more clearly distinguished in comparison to conventional TVs. Quantum dot display show a **wide range of colors more accurately**.

Credit: Nanosysinc.com

3-D Isotropic oscillator

3-D Isotropic oscillator



- The potential of the 3-D isotropic oscillator:

$$\begin{aligned} V(x, y, z) &= \frac{1}{2}m\omega^2 r^2 = \frac{1}{2}m\omega^2 (x^2 + y^2 + z^2) \\ &= V(x) + V(y) + V(z) \end{aligned}$$

- Like particle in a box, we have 3 identical equations to solve in 3-D:

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) &= E_x\phi(x) \\ -\frac{\hbar^2}{2m} \frac{d^2\eta(y)}{dy^2} + V(y)\eta(y) &= E_y\eta(y) \\ -\frac{\hbar^2}{2m} \frac{d^2\zeta(z)}{dz^2} + V(z)\zeta(z) &= E_z\zeta(z) \end{aligned}$$

3-D Isotropic oscillator

- Energy eigenvalues are

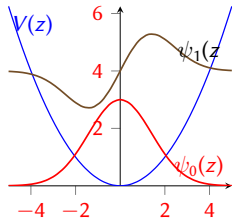
$$E_{n_x, n_y, n_z} = \hbar\omega \left(n_x + n_y + n_z + \frac{3}{2} \right) \quad n_x, n_y, n_z \in 0, 1, \dots$$

- Wavefunctions are

$$\psi_{n_x, n_y, n_z}(x, y, z) = \phi_{n_x}(x) \eta_{n_y}(y) \zeta_{n_z}(z) \quad (6)$$

- Ground state is $n_x = n_y = n_z = 0$

$$\psi_{000}(x, y, z) = \left(\frac{\beta^2}{\pi} \right)^{\frac{3}{4}} e^{-\beta^2(x^2+y^2+z^2)/2}; \quad \beta^2 = \frac{m\omega}{\hbar}$$



3-D Isotropic oscillator

n_x	n_y	n_z	n	Degeneracy
0	0	0	0	None
0	0	1	1	Threefold
0	1	0	1	
1	0	0	1	
0	0	2	2	Sixfold
0	2	0	2	
2	0	0	2	
1	1	0	2	
0	1	1	2	
0	1	1	2	Tenfold
			3	

- First excited state can be obtained in 3 different ways:

$$n_x = n_y = 0, n_z = 1; n_x = n_z = 0, n_y = 1; n_x = 1, n_y = n_z = 0$$

Like earlier example, corresponding ψ 's are different

$$\psi_{100}(x, y, z) = \left(\frac{\beta^2}{\pi}\right)^{\frac{3}{4}} \sqrt{2}(\beta x) e^{-\beta^2(x^2+y^2+z^2)/2}$$

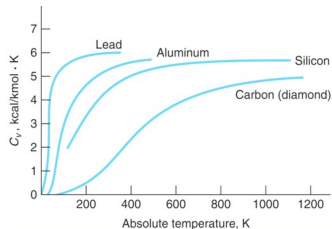
$$\psi_{010}(x, y, z) = \left(\frac{\beta^2}{\pi}\right)^{\frac{3}{4}} \sqrt{2}(\beta y) e^{-\beta^2(x^2+y^2+z^2)/2}$$

$$\psi_{001}(x, y, z) = \left(\frac{\beta^2}{\pi}\right)^{\frac{3}{4}} \sqrt{2}(\beta z) e^{-\beta^2(x^2+y^2+z^2)/2}$$

- Unlike particle in box, except ground state, all excited states are **Degenerate states**

“Real world” Isotropic HO

Dulong-Petit law



Dulong-Petit law is not always true, and is never true at low temperatures!

- Heat capacity (C) of a substance is a measure of how much heat is required to raise the temperature of the substance by one degree Kelvin.
- Dulong and Petit law:** For a solid, the heat capacity is

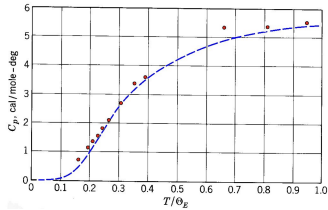
$$C_V = 3k_B \quad \Rightarrow \quad E = 3 k_B T \quad (6)$$

- Classical Interpretation:** From Hooke's law, we can express the proportionality between the deformations of a solid and the counter forces. The energy of an atom in solid

$$E = \frac{1}{2m} \left(p_x^2 + p_y^2 + p_z^2 \right) + \frac{1}{2} m \omega^2 (x^2 + y^2 + z^2)$$

Suppose each degree of freedom has $\epsilon = k_B T / 2$ (**Equipartition law**) leads to (6).

Einstein model of solids (1907 before Schroedinger equation)



Comparison of experimental values of C_V for diamond with values calculated for Einstein model.

- Dulong-Petit law uses the classical description of lattice vibrations. They fail to describe at low temperatures.
- Einstein's model takes into account quantum description of lattice vibrations.
- **Assumption:** Solid is made of N independent 3-D quantum oscillator all with same mass m and frequency ω :

$$E_{\text{total}} = \sum_{i=1}^N \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) + \frac{1}{2} m \omega^2 (x^2 + y^2 + z^2)$$

- Einstein's model was a good attempt to explain the specific heat of solids. However, it could not explain because it assumed that all the normal modes have the same frequency. Debye model overcame this.

Hydrogen atom

Hydrogen Atom: Classical analysis

- Hydrogen atom is the simplest atom in nature. Consists of a negatively charged electron moving around a positively charged proton.



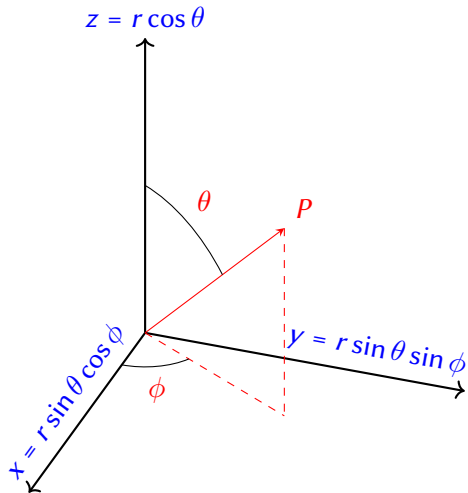
- In Bohr's model, the electron is pulled around the proton in a perfectly circular orbit by an attractive Coulomb potential:

$$V(r) = -\frac{1}{4\pi\epsilon_0} \frac{e}{r} \quad r \text{ is radial distance between proton and electron}$$

- Proton is approximately 1800 times more massive than the electron, so the proton moves very little in response to the force on the proton by the electron. Like Sun-Earth system, Sun moves very little in response to Earth's force.
- We assume Proton to be at rest. Treat Hydrogen as a single particle (electron).

$$T_e = \frac{p^2}{2m_e}; \quad V(r) = -\frac{1}{4\pi\epsilon_0} \frac{e}{r} \quad (7)$$

A bit on coordinate systems



- Coloumb potential is

$$V(x, y, z) = \frac{C_0}{r} = \frac{C_0}{\sqrt{x^2 + y^2 + z^2}}$$

$$\Rightarrow V(x, y, z) \neq V(x) + V(y) + V(z)$$

- For such potentials, Cartesian coordinate (x, y, z) is not useful **Spherical polar** is better suited.
- Transformation between Cartesian and Polar:

$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$

Hydrogen Atom: Quantum Analysis

- Since potential depends only on r , ψ can be written as a product of three functions:

$$\psi_{n,l,m}(r, \theta, \phi) = \underbrace{R_{n,l}(r)}_{\text{Radial func}} \underbrace{\Theta_{l,m}(\theta)}_{\text{Polar func}} \underbrace{\Phi_m(\phi)}_{\text{Angular func}} ; \quad E_n = - \left(\frac{m_e e^4}{8h^2 \epsilon_0^2} \right) \frac{1}{n^2} = - \frac{E_0}{n^2}$$

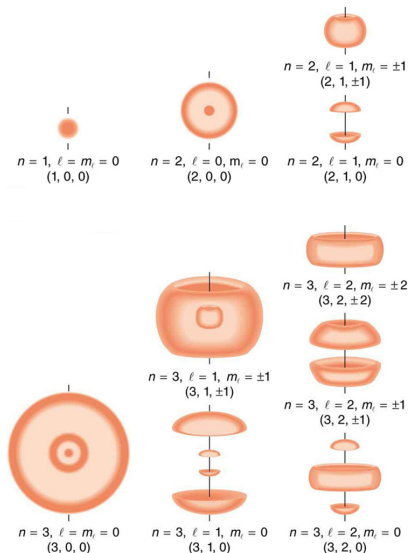
- Quantum numbers (n, l, m) :

n :	principal quantum number	$1, 2, 3, \dots$
l :	angular momentum quantum number	$0, 1, 2, \dots (n-1)$
m :	angular momentum projection quantum number	$-l, -(l+1), \dots, 0, \dots (l-1), l$

- Ground state is unique and is given by $n = 1, l = 0, m = 0$.
- First excited state ($n = 2$) can be obtained in 4 (n^2) different ways (4 degenerate states)

$$l = 0, m = 0; l = 1, m = -1, 0, 1$$

Hydrogen Atom: Quantum Analysis



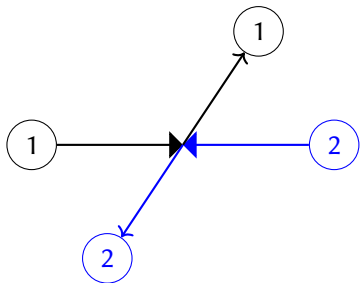
- Probability for the electron in the ground state ($n = 1$) and excited states of hydrogen.
- The probability of finding the electron is indicated by the shade of color; the darker the coloring the greater the chance of finding the electron.
- The nature of these states is determined by their sets of quantum numbers (n, l, m).

Credit: OpenStax

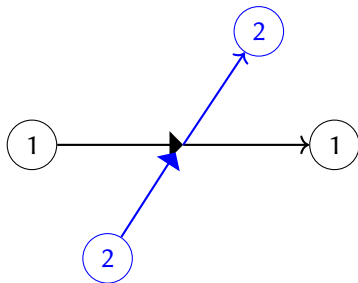
Three types of physical systems

Indistinguishability and the Quantum

Consider the scattering between two identical particles of gas:

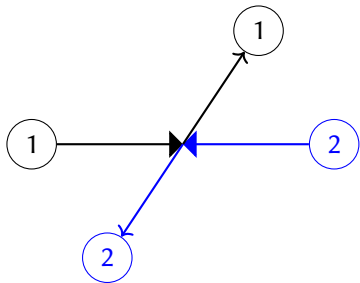


Configuration I of two-particles scattering

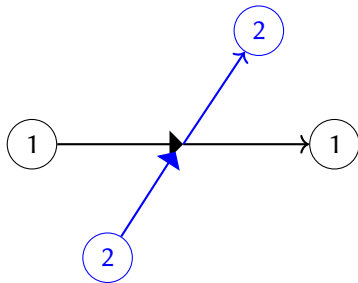


Configuration II of two-particles scattering

Indistinguishability and the Quantum



Configuration I of two-particles scattering

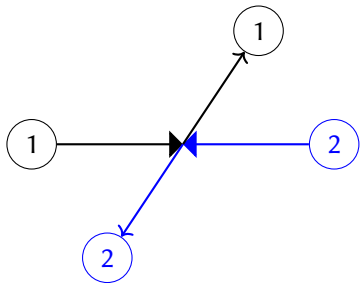


Configuration II of two-particles scattering

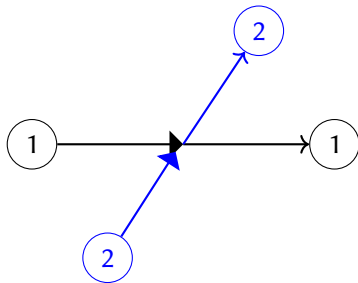
We can treat the scattering of the gas particles in two ways:

- 1 Classical mechanics
- 2 Quantum mechanics

Indistinguishability and the Quantum



Configuration I of two-particles scattering



Configuration II of two-particles scattering

Classical mechanics

Even if they are identical, we can track the two particles continuously and can find which one of the scattering processes occurred.

Quantum mechanics

- Due to Uncertainty principle, such a tracking of particles is not possible!
- If we try to watch the trajectories of the particles, at the crucial time **when the two atoms are nearby**, the uncertainty in the position of the atom is larger, and lose track.
- Since, we can not specify the position and momentum precisely, we will **never be able to know precisely** which of the two events occur.

Indistinguishability and the Quantum

- At an instant of time, consider two particles at positions \mathbf{r}_1 and \mathbf{r}_2 . $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ describes the two particle system.
- The wave function for a system of identical particles must reflect the requirement that the particles are indistinguishable from each other.
- The probability density of the two particle wave function $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ must be identical to that of the the wave function $\Psi(\mathbf{r}_2, \mathbf{r}_1)$ where the particles have been interchanged, i. e.

$$|\Psi(\mathbf{r}_1, \mathbf{r}_2)|^2 = |\Psi(\mathbf{r}_2, \mathbf{r}_1)|^2 .$$

- Two physical relevant cases in 3D are [when we exchange again the square should be 1.]
 - ① Symmetric case: $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \Psi(\mathbf{r}_2, \mathbf{r}_1)$
 - ② Anti-symmetric case: $\Psi(\mathbf{r}_1, \mathbf{r}_2) = -\Psi(\mathbf{r}_2, \mathbf{r}_1)$

Symmetric and Anti-symmetric case

Symmetric case

- $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \Psi(\mathbf{r}_2, \mathbf{r}_1)$
- Such particles are called **Bosons**
- Such Particles have integral or zero intrinsic spin.
- Example: Photons
- Any number of Bosons can occupy the same quantum state

Anti-symmetric case

- $\Psi(\mathbf{r}_1, \mathbf{r}_2) = -\Psi(\mathbf{r}_2, \mathbf{r}_1)$
- Such particles are called **Fermions**
- Such Particles have half-integral intrinsic spin.
- Example: Electrons, Protons, Neutrons
- No two Fermions can occupy the same state \Rightarrow Pauli exclusion principle.

Three types of physical systems

Physical systems in the nature can be classified into three categories:

- Distinguishable particles

- ① Treat the particles as classical billiard balls.
- ② Each of the particles are distinguishable from one another
- ③ Any number of the particles can occupy a single quantum state.

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- Indistinguishable particles whose wavefunctions are Anti-symmetric under exchange

- 1 Indistinguishable particles (Fermions)
- 2 Obey Pauli exclusion principle
- 3 Particles with half-integer spins.

- Indistinguishable particles whose wavefunctions are Symmetric under exchange

- 1 Indistinguishable particles (Bosons)
- 2 Do not obey Pauli exclusion principle
- 3 Particles with integer spins.

Multi-electron atoms

Periodic table and Properties of multi-electron atoms

PERIODIC TABLE

Atomic Properties of the Elements

NIST National Institute of Standards and Technology
U.S. Department of Commerce

FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS¹

¹ second = 9 162 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³Cs

speed of light in vacuum	c	299 792 458 m s ⁻¹	(exact)
Planck constant	h	6.626 070 15 × 10 ⁻³⁴ J Hz ⁻¹	(exact)
elementary charge	e	1.602 176 634 × 10 ⁻¹⁹ C	(exact)
Avogadro constant	N_A	6.022 140 76 × 10 ²³ mol ⁻¹	(exact)
Boltzmann constant	k	1.380 649 × 10 ⁻²³ J K ⁻¹	(exact)
electron volt	eV	1.602 176 634 × 10 ⁻¹⁹ J	(exact)
electron mass	m_e	9.109 383 71 × 10 ⁻³¹ kg	(exact)
energy equivalent	$m_e c^2$	0.510 998 950 MeV	(exact)
proton mass	m_p	1.672 621 894 × 10 ⁻²⁷ kg	(exact)
energy equivalent	$m_p c^2$	938.272 081 MeV	(exact)
fine-structure constant	α	1/137.035 999 074	(exact)
Rydberg energy	R_∞	13.605 693 1230 eV	(exact)
Newtonian constant of gravitation	G	6.674 × 10 ⁻¹¹ m ³ kg ⁻¹ s ⁻²	(exact)

²For the most accurate values of these and other constants, visit nist.gov/constants.

☐ Solids
☐ Liquids
☐ Gases
☐ Artificially Prepared

Physical Measurement Laboratory www.nist.gov/pml
Standard Reference Data www.nist.gov/srd

Period

Group

Symbol

Name

Standard Atomic Weight

Ground-state Configuration

Ionization Energy (eV)

Group	1 IA	2 IIA	FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS ¹										Physical Measurement Laboratory www.nist.gov/pml Standard Reference Data www.nist.gov/srd										18 VIIIA												
1	H 1.008 1s 13.9984	2	He 4.0026 1s 24.5874	3	Li 6.941 2s 5.3917	4	Be 9.0122 2s 9.3227	5	B 10.81 2s 9.3227	6	C 12.011 2s 10.2639	7	N 14.007 2s 14.5285	8	O 15.999 2s 15.8351	9	F 18.998 2s 17.4228	10	Ne 20.180 2s 21.5645	11	Na 22.990 3s 5.1391	12	Mg 24.305 3s 7.3442	13	Al 26.982 3p 5.9858	14	Si 28.086 3p 10.4867	15	P 30.974 3p 10.4867	16	S 32.06 3p 10.4867	17	Cl 35.45 3p 12.9676	18	Ar 39.948 3p 15.7596
2	19 K 39.098 4s 4.1881	20 Ca 40.078 4s 6.1132	21	Sc 44.956 3d 6.5615	22	Ti 47.887 3d 6.9281	23	V 50.942 3d 6.7462	24	Cr 51.996 3d 6.7695	25	Mn 54.938 3d 7.4340	26	Fe 55.845 3d 7.9025	27	Co 58.933 3d 7.8810	28	Ni 58.693 3d 7.6399	29	Cu 63.546 3d 7.7264	30	Zn 65.38 3d 9.3942	31	Ga 69.723 4p 5.9993	32	Ge 72.630 4p 7.8964	33	As 74.922 4p 9.7886	34	Se 78.971 4p 9.7524	35	Br 79.904 4p 11.8158	36	Kr 83.796 4p 13.9999	
3	37 Rb 85.468 5s 4.1771	38 Sr 87.62 5s 5.6949	39	Y 88.906 4d 6.2173	40	Zr 91.224 4d 6.8341	41	Nb 92.906 4d 6.7569	42	Mo 95.94 4d 7.1194	43	Tc 98.906 4d 7.1194	44	Ru 101.07 4d 7.3055	45	Rh 102.91 4d 7.4589	46	Pd 106.42 4d 8.3369	47	Ag 107.87 4d 7.5782	48	Cd 112.41 4d 8.9639	49	In 114.82 5p 7.3439	50	Sn 118.71 5p 8.6934	51	Sb 121.76 5p 9.0007	52	Te 127.60 5p 9.0007	53	I 126.905 5p 10.4513	54	Xe 131.29 5p 12.1298	
4	55 Cs 132.91 6s 3.8939	56 Ba 137.33 6s 5.2117	57	La 138.91 5d 6.8251	58	Ce 140.12 5d 7.4466	59	Pr 140.91 5d 7.9643	60	Nd 144.24 5d 7.9643	61	Pm 144.91 5d 8.3369	62	Sm 150.36 5d 8.4382	63	Eu 151.96 5d 8.4382	64	Gd 157.25 5d 8.9639	65	Tb 158.93 5d 9.0007	66	Dy 162.50 5d 9.0007	67	Ho 164.93 5d 9.0007	68	Er 167.26 5d 9.0007	69	Tm 168.93 5d 9.0007	70	Yb 173.05 5d 9.0007	71	Lu 174.97 5d 9.0007			
5	87 Fr 223.02 7s 4.0727	88 Ra 226.02 7s 5.2174	89	Ac 227.03 6d 6.8251	90	Th 232.04 6d 6.8251	91	Pa 231.04 6d 6.8251	92	U 238.03 6d 6.8251	93	Np 237.04 6d 6.8251	94	Pu 239.04 6d 6.8251	95	Am 243.06 6d 6.8251	96	Cm 247.07 6d 6.8251	97	Bk 247.07 6d 6.8251	98	Cf 251.08 6d 6.8251	99	Es 252.08 6d 6.8251	100	Fm 257.10 6d 6.8251	101	Md 258.10 6d 6.8251	102	No 259.10 6d 6.8251	103	Lr 262.10 6d 6.8251			
6	104 Rf 101.07 6d 6.8251	105 Db 102.91 6d 6.8251	106	Sg 106.42 6d 6.8251	107	Bh 107.87 6d 6.8251	108	Hs 112.41 6d 6.8251	109	Mt 114.82 6d 6.8251	110	Ds 118.71 6d 6.8251	111	Rg 121.76 6d 6.8251	112	Cn 127.60 6d 6.8251	113	Nh 126.905 6d 6.8251	114	Fl 127.60 6d 6.8251	115	Mc 126.905 6d 6.8251	116	Lv 126.905 6d 6.8251	117	Ts 126.905 6d 6.8251	118	Og 126.905 6d 6.8251							
7	131 Nh 286 7s 6.8251	132 Fl 289 7s 6.8251	133	Mc 289 7s 6.8251	134	Lv 289 7s 6.8251	135	Ts 289 7s 6.8251	136	Og 289 7s 6.8251	137	Bohrium 289 7s 6.8251	138	Hassium 289 7s 6.8251	139	Meitnerium 289 7s 6.8251	140	Darmstadtium 289 7s 6.8251	141	Roentgenium 289 7s 6.8251	142	Copernicium 289 7s 6.8251	143	Nihonium 289 7s 6.8251	144	Flerovium 289 7s 6.8251	145	Moscovium 289 7s 6.8251	146	Livermorium 289 7s 6.8251	147	Tennessine 289 7s 6.8251	148	Oganesson 289 7s 6.8251	
8	149 Nh 286 7s 6.8251	150 Fl 289 7s 6.8251	151	Mc 289 7s 6.8251	152	Lv 289 7s 6.8251	153	Ts 289 7s 6.8251	154	Og 289 7s 6.8251	155	Bohrium 289 7s 6.8251	156	Hassium 289 7s 6.8251	157	Meitnerium 289 7s 6.8251	158	Darmstadtium 289 7s 6.8251	159	Roentgenium 289 7s 6.8251	160	Copernicium 289 7s 6.8251	161	Nihonium 289 7s 6.8251	162	Flerovium 289 7s 6.8251	163	Moscovium 289 7s 6.8251	164	Livermorium 289 7s 6.8251	165	Tennessine 289 7s 6.8251	166	Oganesson 289 7s 6.8251	

¹Based upon ¹²C. (i) indicates the mass number of the longest-lived isotope.

For the most precise values and uncertainties visit ciaw.org and pml.nist.gov/pml.

NIST SP 966 (July 2019)

- All atoms **except Hydrogen** are multiple-electron atoms.
- The physical and chemical properties of elements are related to the number of electrons a neutral atom has!
- The periodic table of the elements groups elements with similar properties into columns.
- It is also arranged with increasing number of electrons in a neutral atom (atomic number Z).

¹Based upon ¹³³Cs. (t) indicates the mass number of the longest-lived isotope.

For the most precise values and uncertainties visit ciw.org and pml.nist.gov/data.

NIST SP 966 (July 2019)

Periodic table and Properties of multi-electron atoms

PERIODIC TABLE

Atomic Properties of the Elements

Group	FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS ¹																Physical Measurement Laboratory www.nist.gov/pml										18								
1 IA																	Standard Reference Data www.nist.gov/srd										VIII VIII								
1 H 1.008 1.00784	¹ second = 9192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³ Cs speed of light in vacuum c 299 792 458 m s ⁻¹ (exact) Planck constant h 6.626 070 15 × 10 ⁻³⁴ J s (exact) elementary charge e 1.602 176 634 × 10 ⁻¹⁹ C (exact) Avogadro constant N_A 6.022 140 76 × 10 ²³ mol ⁻¹ (exact) Boltzmann constant k 1.380 658 × 10 ⁻²³ J K ⁻¹ (exact) electron volt eV 1.602 176 634 × 10 ⁻¹⁹ J (exact) electron mass $m_e c^2$ 0.510 998 950 MeV (exact) proton mass $m_p c^2$ 938.272 088 MeV (exact) fine-structure constant α 1/137.035 999 (exact) Rydberg energy R_∞ 13.605 693 1230 eV (exact) Newtonian constant of gravitation G 6.674 × 10 ⁻¹¹ m ³ kg ⁻¹ s ⁻² (exact)																[†] For the most accurate values of these and other constants, visit nist.gov/constants . Solids Liquids Gases Artificially Prepared										2 He 4.0026 4.002602								
2 Li 6.94 6.941 3.0917	3 Be 9.0122 9.012182															13 Al 26.9815385 26.9815386	14 Si 28.0855836 28.0855835	15 P 30.973761998 30.973761998	16 S 32.065 32.065	17 Cl 35.453 35.453	18 Ar 39.948 39.948														
3 Na 22.98976928 22.98976928	4 Mg 24.304 24.304	5 Al 26.9815385 26.9815386	6 Si 28.0855836 28.0855835	7 P 30.973761998 30.973761998	8 S 32.065 32.065	9 Cl 35.453 35.453	10 Ar 39.948 39.948	11 K 39.0983 39.0983	12 Ca 40.078 40.078	13 Sc 44.9559122 44.9559122	14 Ti 47.88 47.88	15 V 50.9415 50.9415	16 Cr 51.9961 51.9961	17 Mn 54.938044 54.938044	18 Fe 55.845 55.845	19 Co 58.933194 58.933194	20 Ni 58.6934 58.6934	21 Cu 63.546 63.546	22 Zn 65.38 65.38	23 Ga 69.723 69.723	24 Ge 72.630 72.630	25 As 74.9216 74.9216	26 Se 78.96 78.96	27 Br 79.904 79.904	28 Kr 83.798 83.798										
4 K 39.0983 39.0983	5 Ca 40.078 40.078	6 Sc 44.9559122 44.9559122	7 Ti 47.88 47.88	8 V 50.9415 50.9415	9 Cr 51.9961 51.9961	10 Mn 54.938044 54.938044	11 Fe 55.845 55.845	12 Co 58.933194 58.933194	13 Ni 58.6934 58.6934	14 Cu 63.546 63.546	15 Zn 65.38 65.38	16 Ga 69.723 69.723	17 Ge 72.630 72.630	18 As 74.9216 74.9216	19 Se 78.96 78.96	20 Br 79.904 79.904	21 Kr 83.798 83.798	22 Rb 85.468 85.468	23 Sr 87.62 87.62	24 Y 88.90584 88.90584	25 Zr 91.224 91.224	26 Nb 92.90638 92.90638	27 Mo 95.94 95.94	28 Tc 98.90625 98.90625	29 Ru 101.07 101.07	30 Rh 101.07 101.07	31 Pd 106.42 106.42	32 Ag 107.8682 107.8682	33 Cd 112.411 112.411	34 In 114.818 114.818	35 Sn 118.710 118.710	36 Sb 121.757 121.757	37 Te 127.60 127.60	38 I 126.90547 126.90547	39 Xe 131.29 131.29
5 Rb 85.468 85.468	6 Sr 87.62 87.62	7 Y 88.90584 88.90584	8 Zr 91.224 91.224	9 Nb 92.90638 92.90638	10 Mo 95.94 95.94	11 Tc 98.90625 98.90625	12 Ru 101.07 101.07	13 Rh 101.07 101.07	14 Pd 106.42 106.42	15 Ag 107.8682 107.8682	16 Cd 112.411 112.411	17 In 114.818 114.818	18 Sn 118.710 118.710	19 Sb 121.757 121.757	20 Te 127.60 127.60	21 I 126.90547 126.90547	22 Xe 131.29 131.29	23 Ba 137.327 137.327	24 La 138.90547 138.90547	25 Ce 140.12 140.12	26 Pr 140.90765 140.90765	27 Nd 144.242 144.242	28 Pm 144.91274 144.91274	29 Sm 150.36 150.36	30 Eu 151.964 151.964	31 Gd 157.25 157.25	32 Tb 158.92534 158.92534	33 Dy 162.50031 162.50031	34 Ho 164.93032 164.93032	35 Er 167.259 167.259	36 Tm 168.93002 168.93002	37 Yb 173.0547 173.0547	38 Lu 174.967 174.967		
6 Cs 132.905451963 132.905451963	7 Ba 137.327 137.327	8 La 138.90547 138.90547	9 Ce 140.12 140.12	10 Pr 140.90765 140.90765	11 Nd 144.242 144.242	12 Pm 144.91274 144.91274	13 Sm 150.36 150.36	14 Eu 151.964 151.964	15 Gd 157.25 157.25	16 Tb 158.92534 158.92534	17 Dy 162.50031 162.50031	18 Ho 164.93032 164.93032	19 Er 167.259 167.259	20 Tm 168.93002 168.93002	21 Yb 173.0547 173.0547	22 Lu 174.967 174.967	23 Hf 178.49 178.49	24 Ta 180.94788 180.94788	25 W 183.84 183.84	26 Re 186.207 186.207	27 Os 190.23 190.23	28 Ir 192.222 192.222	29 Pt 195.084 195.084	30 Au 196.966569 196.966569	31 Hg 200.59 200.59	32 Tl 204.38 204.38	33 Pb 207.2 207.2	34 Bi 208.980399 208.980399	35 Po 209 209	36 At 210 210	37 Rn 222 222	38 Fr 223 223	39 Ra 226 226		
7 Fr 223 223	8 Ra 226 226	9 Ac 227 227	10 Th 232.0377 232.0377	11 Pa 231.036889 231.036889	12 U 238.02891 238.02891	13 Np 237.048173 237.048173	14 Pu 244.064224 244.064224	15 Am 243.061381 243.061381	16 Cm 247 247	17 Bk 247 247	18 Cf 251 251	19 Es 252 252	20 Fm 257 257	21 Md 258 258	22 No 259 259	23 Lr 262 262	24 Th 232.0377 232.0377	25 Pa 231.036889 231.036889	26 U 238.02891 238.02891	27 Np 237.048173 237.048173	28 Pu 244.064224 244.064224	29 Am 243.061381 243.061381	30 Cm 247 247	31 Bk 247 247	32 Cf 251 251	33 Es 252 252	34 Fm 257 257	35 Md 258 258	36 No 259 259	37 Lr 262 262					
8 Fr 223 223	9 Ra 226 226	10 Ac 227 227	11 Th 232.0377 232.0377	12 Pa 231.036889 231.036889	13 U 238.02891 238.02891	14 Np 237.048173 237.048173	15 Pu 244.064224 244.064224	16 Am 243.061381 243.061381	17 Cm 247 247	18 Bk 247 247	19 Cf 251 251	20 Es 252 252	21 Fm 257 257	22 Md 258 258	23 No 259 259	24 Lr 262 262	25 Th 232.0377 232.0377	26 Pa 231.036889 231.036889	27 U 238.02891 238.02891	28 Np 237.048173 237.048173	29 Pu 244.064224 244.064224	30 Am 243.061381 243.061381	31 Cm 247 247	32 Bk 247 247	33 Cf 251 251	34 Es 252 252	35 Fm 257 257	36 Md 258 258	37 No 259 259	38 Lr 262 262					
9 Fr 223 223	10 Ra 226 226	11 Ac 227 227	12 Th 232.0377 232.0377	13 Pa 231.036889 231.036889	14 U 238.02891 238.02891	15 Np 237.048173 237.048173	16 Pu 244.064224 244.064224	17 Am 243.061381 243.061381	18 Cm 247 247	19 Bk 247 247	20 Cf 251 251	21 Es 252 252	22 Fm 257 257	23 Md 258 258	24 No 259 259	25 Lr 262 262	26 Th 232.0377 232.0377	27 Pa 231.036889 231.036889	28 U 238.02891 238.02891	29 Np 237.048173 237.048173	30 Pu 244.064224 244.064224	31 Am 243.061381 243.061381	32 Cm 247 247	33 Bk 247 247	34 Cf 251 251	35 Es 252 252	36 Fm 257 257	37 Md 258 258	38 No 259 259	39 Lr 262 262					
10 Fr 223 223	11 Ra 226 226	12 Ac 227 227	13 Th 232.0377 232.0377	14 Pa 231.036889 231.036889	15 U 238.02891 238.02891	16 Np 237.048173 237.048173	17 Pu 244.064224 244.064224	18 Am 243.061381 243.061381	19 Cm 247 247	20 Bk 247 247	21 Cf 251 251	22 Es 252 252	23 Fm 257 257	24 Md 258 258	25 No 259 259	26 Lr 262 262	27 Th 232.0377 232.0377	28 Pa 231.036889 231.036889	29 U 238.02891 238.02891	30 Np 237.048173 237.048173	31 Pu 244.064224 244.064224	32 Am 243.061381 243.061381	33 Cm 247 247	34 Bk 247 247	35 Cf 251 251	36 Es 252 252	37 Fm 257 257	38 Md 258 258	39 No 259 259	40 Lr 262 262					
11 Fr 223 223	12 Ra 226 226	13 Ac 227 227	14 Th 232.0377 232.0377	15 Pa 231.036889 231.036889	16 U 238.02891 238.02891	17 Np 237.048173 237.048173	18 Pu 244.064224 244.064224	19 Am 243.061381 243.061381	20 Cm 247 247	21 Bk 247 247	22 Cf 251 251	23 Es 252 252	24 Fm 257 257	25 Md 258 258	26 No 259 259	27 Lr 262 262	28 Th 232.0377 232.0377	29 Pa 231.036889 231.036889	30 U 238.02891 238.02891	31 Np 237.048173 237.048173	32 Pu 244.064224 244.064224	33 Am 243.061381 243.061381	34 Cm 247 247	35 Bk 247 247	36 Cf 251 251	37 Es 252 252	38 Fm 257 257	39 Md 258 258	40 No 259 259	41 Lr 262 262					
12 Fr 223 223	13 Ra 226 226	14 Ac 227 227	15 Th 232.0377 232.0377	16 Pa 231.036889 231.036889	17 U 238.02891 238.02891	18 Np 237.048173 237.048173	19 Pu 244.064224 244.064224	20 Am 243.061381 243.061381	21 Cm 247 247	22 Bk 247 247	23 Cf 251 251	24 Es 252 252	25 Fm 257 257	26 Md 258 258	27 No 259 259	28 Lr 262 262	29 Th 232.0377 232.0377	30 Pa 231.036889 231.036889	31 U 238.02891 238.02891	32 Np 237.048173 237.048173	33 Pu 244.064224 244.064224	34 Am 243.061381 243.061381	35 Cm 247 247	36 Bk 247 247	37 Cf 251 251	38 Es 252 252	39 Fm 257 257	40 Md 258 258	41 No 259 259	42 Lr 262 262					
13 Fr 223 223	14 Ra 226 226	15 Ac 227 227	16 Th 232.0377 232.0377	17 Pa 231.036889 231.036889	18 U 238.02891 238.02891	19 Np 237.048173 237.048173	20 Pu 244.064224 244.064224	21 Am 243.061381 243.061381	22 Cm 247 247	23 Bk 247 247	24 Cf 251 251	25 Es 252 252	26 Fm 257 257	27 Md 258 258	28 No 259 259	29 Lr 262 262	30 Th 232.0377 232.0377	31 Pa 231.036889 231.036889	32 U 238.02891 238.02891	33 Np 237.048173 237.048173	34 Pu 244.064224 244.064224	35 Am 243.061381 243.061381	36 Cm 247 247	37 Bk 247 247	38 Cf 251 251	39 Es 252 252	40 Fm 257 257	41 Md 258 258	42 No 259 259	43 Lr 262 262					
14 Fr 223 223	15 Ra 226 226	16 Ac 227 227	17 Th 232.0377 232.0377	18 Pa 231.036889 231.036889	19 U 238.02891 238.02891	20 Np 237.048173 237.048173	21 Pu 244.064224 244.064224	22 Am 243.061381 243.061381	23 Cm 247 247	24 Bk 247 247	25 Cf 251 251	26 Es 252 252	27 Fm 257 257	28 Md 258 258	29 No 259 259	30 Lr 262 262	31 Th 232.0377 232.0377	32 Pa 231.036889 231.036889	33 U 238.02891 238.02891	34 Np 237.048173 237.048173	35 Pu 244.064224 244.064224	36 Am 243.061381 243.061381	37 Cm 247 247	38 Bk 247 247	39 Cf 251 251	40 Es 252 252	41 Fm 257 257	42 Md 258 258	43 No 259 259	44 Lr 262 262					
15 Fr 223 223	16 Ra 226 226	17 Ac 227 227	18 Th 232.0377 232.0377	19 Pa 231.036889 231.036889	20 U 238.02891 238.02891	21 Np 237.048173 237.048173	22 Pu 244.064224 244.064224	23 Am 243.061381 243.061381	24 Cm 247 247	25 Bk 247 247	26 Cf 251 251	27 Es 252 252	28 Fm 257 257	29 Md 258 258	30 No 259 259	31 Lr 262 262	32 Th 232.0377 232.0377	33 Pa 231.036889 231.036889	34 U 238.02891 238.02891	35 Np 237.048173 237.048173	36 Pu 244.064224 244.064224	37 Am 243.061381 243.061381	38 Cm 247 247	39 Bk 247 247	40 Cf 251 251	41 Es 252 252	42 Fm 257 257	43 Md 258 258	44 No 259 259	45 Lr 262 262					
16 Fr 223 223	17 Ra 226 226	18 Ac 227 227	19 Th 232.0																																

Key Take-aways

- In 1-D, particle can move in only forward or backward direction. In 3-D, particles can choose to move in infinite directions!
- Depending on the form of the potential, we can have many quantum states that have the same energy eigenvalue — Degeneracy of states \Rightarrow Existence of symmetry
- We have explicitly show the degeneracy for particle in 3-D box and isotropic oscillator.
If box size is not the same, the degeneracy decreases in particle in 3-D box.
- Like in 1-D, the ground state energy is greater than zero. The stationary states (states of definite energy) have non-zero values also in regions beyond classical turning points.
- Looked at application of model 3-D systems to real world!