



# Lecture #1

February 7

---

Syllabus and general course information.

Review: How does one solve the Schrödinger equation?

Example: hydrogen-like atom.

Special hydrogenic systems: positronium, muonium, antihydrogen, muonic and hadronic atoms.



# Lecture #1

February 8

Chapters 7.2, 7.5 pages 336-341, 351-357, Bransden & Joachain,  
Quantum Mechanics

Lectures on Atomic Physics, Walter Johnson, p. 25 -31 (Complete  
lectures are available online; printed version is at the library)



# Quantum Mechanics 812

---

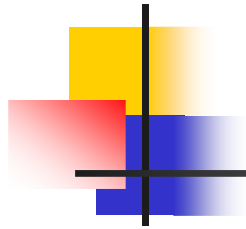
Course will introduce both fundamental concepts and techniques of quantum mechanics and demonstrate their relevance to real-life modern applications



# Goals of the course

---

- Learn fundamentals of quantum mechanics
- Learn how quantum mechanics is relevant to research in various fields and today's technology
- Aid in student's research or in selection of field research
- ...



# Learning

---

The objective of the course is not to cover certain set of topics but to provide a base of fundamentals concepts and skills as well as to demonstrate examples of their applications which will facilitate further interest, learning, and thinking.



# Textbooks

---

- *Quantum mechanics*, B.H. Bransden and C.J. Joachain (second edition)
- Other textbooks:
- *Quantum Mechanics: Fundamentals & Applications to Technology*, by Jasprit Singh
  - *Lecture notes on Atomic Physics*, by Walter Johnson; available online at <http://www.nd.edu/~johnson> under “Unpublished material”.
  - *Physics of Atoms and Molecules*, B.H. Bransden and C.J. Joachain (second edition)



# Homework

---

- Homework is assigned ones a week, on Thursday.
- It is due in one week, next Thursday.
- Exceptions will be noted on the assignments
- Late homework policy: it is best to always return it **on time**
- **MAXIMUM** number of late homeworks: **1**  
(no more than a **week** late)
- No explanation or notification is needed
- Homework will be graded



# Grading standard

---

Each problem is graded using “+”, “±”, “∓”, and “–” marks which are assigned in accordance with the following standards:

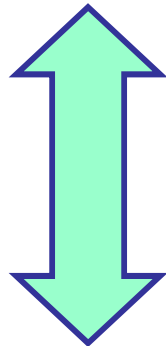
- 3** “+” The problem is solved correctly
- 2** “±” Substantial portion of the solution, which is in the direction of the correct answer is given or complete (in principle correct) solution is given but some mistake is made which lead to incorrect answer.
- 1** “∓” An attempt to solve problem has been made and an understanding of how such problem may be solved is demonstrated (some work in the direction of the correct solution is present).
- 0** “–” No solution is provided or no understanding of how such problem may be solved is demonstrated.



# What does a physical theory involve?

---

Basic physical concepts



Set of rules which map the physical concepts to the corresponding mathematical objects

Mathematical formalism



# How are the problems solved?

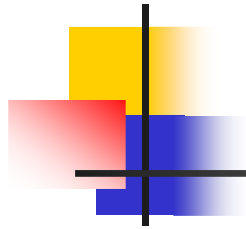
---

Express physical problem in  
mathematical terms

Solve it using mathematical  
techniques

Set of rules which relate mathematical  
formalism to observable reality

Translate mathematical  
solution back into the  
physical world



# Hydrogenic systems

---

What do we want to do: definition of the problem.

Find energy levels and wave functions.

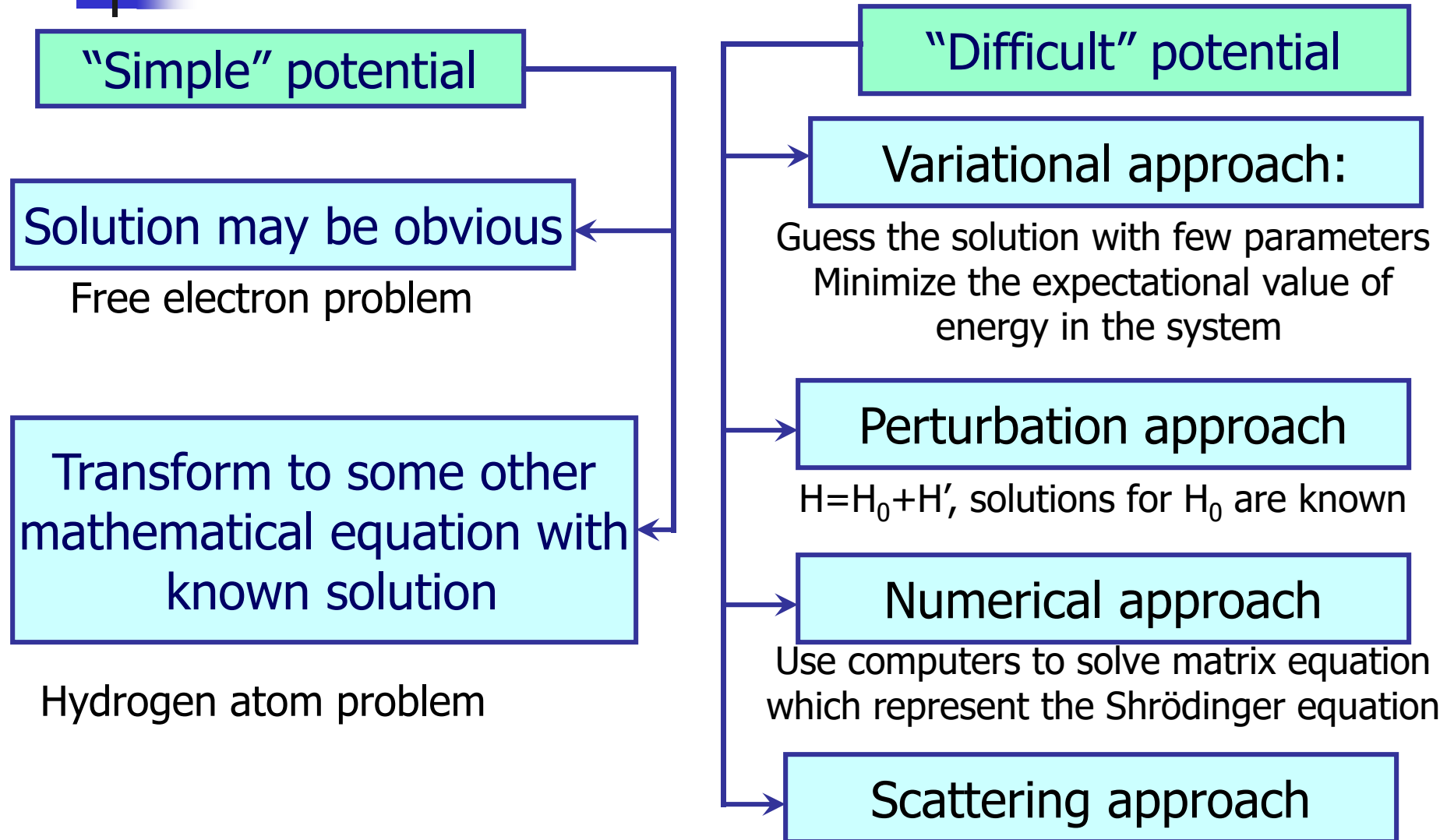
Why wave functions?

Knowledge of the wave functions allows one to calculate atomic properties (various observables).

How to?

Solve the Schrödinger equation.

# How does one solve the Schrödinger equation? (Time independent potential)



Potential  $V(r)$  depends only on radial distance  $r$  from the origin

# Spherically symmetric potential

Electron is moving in a central potential

$$V(r) = V_{nuc}(r) + U(r)$$

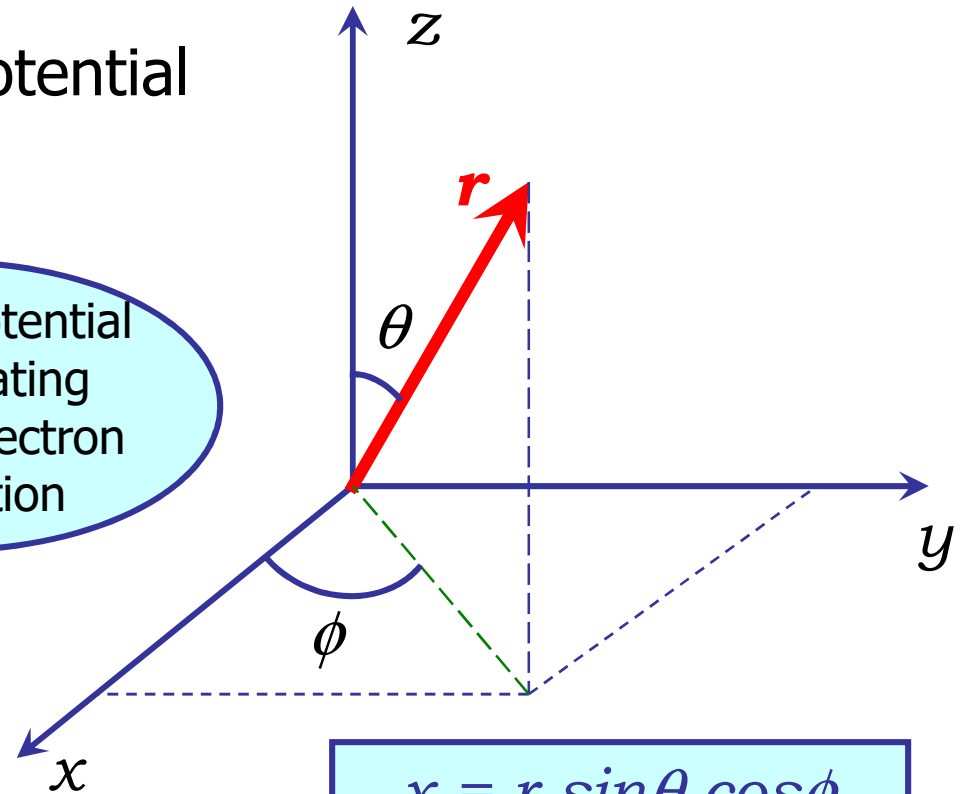
$$-\frac{Ze^2}{4\pi\epsilon_0} \frac{1}{r}$$

Average potential  
approximating  
electron-electron  
interaction

$$H\psi = E\psi$$

$$H = \frac{p^2}{2m} + V(r)$$

$$\mathbf{p} = -i\hbar\nabla$$



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

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

$$z = r \cos\theta$$

# Spherically symmetric potential

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2m}{\hbar^2} (E - V(r)) \psi = 0$$

Separate variables  $\psi(r) = \frac{1}{r} P(r) Y(\theta, \phi)$

If  $\lambda = l(l+1)$   
 $l = 0, 1, 2, \dots \Rightarrow Y_{lm}(\theta, \phi)$   
*spherical harmonics*

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} + \lambda Y = 0$$

$$\frac{d^2 P}{dr^2} + \frac{2m}{\hbar^2} \left( E - V(r) - \frac{\lambda \hbar^2}{2mr^2} \right) P = 0$$

$$\langle A \rangle = \int d^3 r \psi^\dagger(\mathbf{r}) A \psi(\mathbf{r})$$

$$\psi(\mathbf{r}) = \frac{1}{r} P(r) Y_{lm}(\theta, \phi)$$

$$\langle L^2 \rangle = l(l+1) \hbar^2$$

$$\langle L_z \rangle = m_l \hbar$$

# Parity & atomic wave function

$$\psi(\mathbf{r}) = R_{nl}(r)Y_{lm}(\theta, \phi)$$

$$\mathbf{r} \rightarrow -\mathbf{r}$$

$$(r, \theta, \phi) \rightarrow (r, \pi - \theta, \phi + \pi)$$

$R_{nl}(r)$ : *unaffected*

$$Y_{lm}(\theta, \phi) \rightarrow (-1)^l Y_{lm}(\theta, \phi)$$

$$\mathcal{P}[R_{nl}(r)Y_{lm}(\theta, \phi)] = (-1)^l R_{nl}(r)Y_{lm}(\theta, \phi)$$

*Even  $l \rightarrow$  even parity wave function*

*Odd  $l \rightarrow$  odd parity wave function*

<i>s</i>	<i>p</i>	<i>d</i>	<i>f</i>	<i>g</i>
↕	↕	↕	↕	↕
0	1	2	3	4



# Coulomb wave functions

---

$$\frac{d^2 P}{dr^2} + \frac{2m}{\hbar^2} \left( E - \frac{Ze^2}{4\pi\epsilon_0 r} - \frac{l(l+1)\hbar^2}{2mr^2} \right) P = 0$$

Atomic units

$$\hbar = 1$$

$$m_e = 1$$

$$|e| / \sqrt{4\pi\epsilon_0} = 1$$

$$|e| = 1$$

$$4\pi\epsilon_0 = 1$$

Atomic unit of length: Bohr radius

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} = 0.529177 \dots \text{\AA}$$

Atomic unit of energy: Hartree

$$(2\text{Ry}^\infty) = \frac{m_e e^4}{(4\pi\epsilon_0 \hbar)^2} = 27.2114 \dots eV$$





# Coulomb wave functions

---

$$\frac{d^2P}{dr^2} + 2\left(E - \frac{Z}{r} - \frac{l(l+1)}{2r^2}\right)P = 0$$

Atomic units

$$\hbar = 1$$

$$m_e = 1$$

$$|e| / \sqrt{4\pi\epsilon_0} = 1$$

$$|e| = 1$$

$$4\pi\epsilon_0 = 1$$

Atomic unit of length: Bohr radius

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = 0.529177\dots\text{\AA}$$

Atomic unit of energy: Hartree

$$(2\text{Ry}^\infty) = \frac{m_e e^4}{(4\pi\epsilon_0\hbar)^2} = 27.2114\dots eV$$

# Coulomb wave functions

$$\int_0^{\infty} dr P^2(r) = 1$$

$$\frac{d^2 P}{dr^2} + 2 \left( E - \frac{Z}{r} - \frac{l(l+1)}{2r^2} \right) P = 0$$

$$P(r) \xrightarrow{r \rightarrow 0} \begin{cases} r^{l+1} & \text{regular at the origin} \\ r^{-l} & \text{irregular at the origin} \end{cases} \quad \frac{d^2 P}{dr^2} + \frac{l(l+1)}{r^2} P = 0$$

$$P(r) \xrightarrow{r \rightarrow \infty} \begin{cases} e^{-\lambda r} & \text{regular at infinity} \\ e^{\lambda r} & \text{irregular at infinity} \end{cases} \quad \frac{d^2 P}{dr^2} + 2EP = 0 \quad \lambda = \sqrt{-2E}$$

$$P(r) = r^{l+1} e^{-\lambda r} F(r)$$

$$x = 2\lambda r$$

$$x \frac{d^2 F}{dx^2} + (b - x) \frac{dF}{dx} - aF = 0$$

$$a = l + 1 - Z / \lambda$$

$$b = 2(l + 1)$$

*Kummer's equation*

F(x): Confluent Hypergeometric function

F(x): Confluent Hypergeometric function

$$\int_0^{\infty} dr P^2(r) = 1$$

# Coulomb wave functions

$$P(r) = r^{l+1} e^{-\lambda r} F(r)$$

$$x = 2\lambda r$$

$$\lambda = \sqrt{-2E}$$

$$x \frac{d^2 F}{dx^2} - (b-x) \frac{dF}{dx} - aF = 0$$

$$a = l+1 - Z/\lambda$$

$$b = 2(l+1)$$

Kummer's equation

$\Gamma(a) = \infty$  when  $a$  is a **negative integer**  $n_r$

$$F(a, b, x) \xrightarrow{\text{large } |x|} \frac{\Gamma(b)}{\Gamma(a)} e^x x^{a-b} [1 + O(|x|^{-1})]$$

$$a = -n_r$$

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

- The Confluent Hypergeometric function with  $a = -n_r$  reduces to a polynomial of degree  $n_r$ .
- The number  $n_r$  indicated the number of nodes (zeros) of the radial function with  $r > 0$ .

F(x): Confluent Hypergeometric function

# Coulomb wave functions

$$a = -n_r$$
$$n_r = 0, 1, 2, \dots$$

$$a = -n_r = l + 1 - Z / \lambda$$

$$\lambda = \sqrt{-2E}$$

$$E_n = -\frac{Z^2}{2n^2}$$

$$\lambda = \frac{Z}{n_r + l + 1} = \frac{Z}{n}$$

principal quantum number  
 $n = n_r + l + 1$

- There are  $n$  distinct radial functions corresponding to  $E_n$ .
- The number of nodes increases in direct proportion to  $n$  for a fixed  $l$ .
- The outermost maximum of each wave function occurs at increasing distances from the origin as  $n$  increases.
- The value of  $|P_{nl}(r)|^2$  gives the probability that the electron is to be found at a distance  $r$  from the nucleus (regardless of direction.)
- The value of  $|P_{nl}(r)/r|^2$  gives electron density as a function of  $r$  along the given direction.

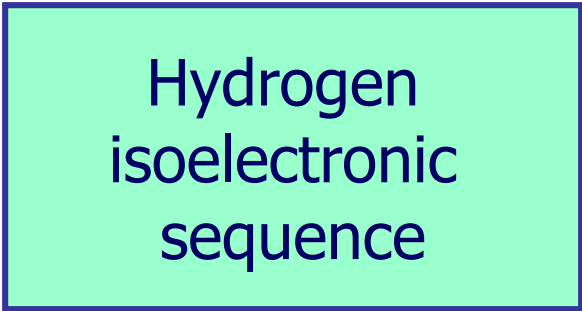


# "Normal" hydrogenic systems

or

Hydrogen-like ions

- He<sup>+</sup> ion (Z=2)
- Li<sup>++</sup> ion (Z=3)
- Be<sup>3+</sup> ion (Z=4)
- ...



Hydrogen  
isoelectronic  
sequence

$$E_n = -\frac{Z^2}{2n^2}, n=1 \Rightarrow I_P = -E_1 = \frac{Z^2}{2}$$

Ionization potential  
increases by  $Z^2$ .



# Isoelectronic sequences

Na  
Z=11

## Sodium-like ions

- Mg<sup>+</sup> ion (Z=12)
- Al<sup>++</sup> ion (Z=13)
- Si<sup>3+</sup> ion (Z=14)
- ...

Sodium  
isoelectronic  
sequence



# Hydrogenic systems: deuterium and tritium.

---

- Deuterium: nucleus contains one proton and one neutron
- Tritium: nucleus contains one proton and two neutrons
- Slightly different reduced mass  $m_e \rightarrow \mu = \frac{m_e M}{M + m_e}$
- Nearly the same ionization potentials ( $10^{-3}$ )
- Slight differences: isotope shifts



# Special hydrogenic systems: positronium & muonium.

---

- Replace nucleus with another particle
- Positronium: bound hydrogenic system made from electron and positron ( $e^+e^-$ ).  
Reduced mass:  $\frac{1}{2}$ , ionisation potential:  $\frac{1}{4}$ .
- Muonium: proton is replaced by a positive muon  $\mu^+$  [ $M \approx 207$ ], ( $\mu^+e^-$ ). Unstable with lifetime  $\tau \approx 2 \times 10^{-6}$  s  
Reduced mass:  $\approx 1$ , ionization potential  $\frac{1}{2}$ .
- Interest: contain only leptons, so they are not affected by strong interactions.
- Particularly suitable to verify the prediction of QED.





# Special hydrogenic systems: antihydrogen. $(\bar{p}e^+)$

---

- Replace proton with antiproton and electron with positron
- First observed in 1996 at CERN (9 atoms, 40ns).
- Reduced mass: 1, ionisation potential:  $\frac{1}{2}$ .
- Interest: to test CPT symmetry



# Special hydrogenic systems: muonic atoms.

---

- Muonic atoms: replace electron with muon
- Reduced mass  $\approx 186$ , ionization potential  $\approx 93$
- and “radius” is 186 times smaller than that of the hydrogen atom.
- Spectral lines in X-ray region (multiply hydrogen frequencies by 186).
- ( $N\mu$ ): Lead,  $Z=82$  can no longer use the previous formulas as we can not consider both particles point-like.
- Interest: to probe the nucleus (energy spectrum is sensitive to internal structure of the nucleus.)



# Special hydrogenic systems: hadronic atoms.

---

- Hadronic atoms: replace electron with hadron (particles which can have strong interactions)
- Strong interactions: can not directly apply theory of hydrogenic systems
- Excited states (especially with  $l > 0$ ) can be studied within this approach as strong interactions have a short range.