Lecture 1 - Introduction

What's important:
- course outline
- review of old quantum theory

Text: Gasiorowicz, Chap. 1

PHYS 385 assumes that the student has completed a 6-7 week introduction to quantum concepts at the second year level and is currently enrolled in a first course on differential equations. The lectures follow the recommended text for much of the course, and an attempt is made to keep the notation consistent with it.

Textbook

Recommended:

Stephen Gasiorowicz *Quantum Physics* (2nd ed.)

Supplementary:

Leonard Schiff, *Quantum Mechanics*

Marking

roughly 10 assignments	15%
midterm exam	25%
final exam	60%

Outline

1. Wave packets and probability
2. Schrödinger equation and its interpretation
3. Review of one-dimensional systems
4. Schrödinger equation in three dimensions
5. Hydrogen atom
6. Spin
7. Time-independent perturbation theory
8. Poly-electron atoms
9. Molecules
10. Collision theory

Introduction

Second year courses on modern physics introduce the idea that the energy of a photon with frequency ν is quantized as

$$E = h\nu \tag{1}$$

where

h = Planck's constant = 6.63×10^{-34} J-s.

This proposal explained two physical phenomena that had challenged physicists at the end of the nineteen century:

- the frequency distribution of electromagnetic radiation in equilibrium at a fixed temperature
- the photoelectric effect.

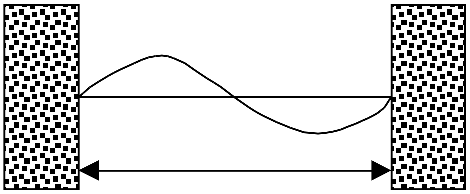
The role of quantized energy in explaining these phenomena is described in all introductory texts on quantum mechanics, and will not be discussed further here. Rather, our starting point is the "old" quantum theory of Bohr and de Broglie, that made analytical predictions for the energy of the hydrogen atom. We do this partly because the predictions are algebraically correct, and partly to highlight the importance of angular momentum in distinguishing between Bohr's and Schrödinger's approaches.

de Broglie wavelength and quantization

From introductory physics, we're familiar with the idea that de Broglie's formula

$$\lambda = h/p \qquad (2)$$

applies to both massless photons and massive particles alike, where λ is the particle's wavelength and p is its momentum. For periodic motion, the stationary states of a system are analogous to the standing waves on a string, with Eq. (2) providing the relevant wavelength. Thus, for a particle moving in one dimension between two hard walls separated by a distance L,



the standing wave condition reads:

$$L = n\lambda/2 \qquad n = 1, 2, 3... \qquad (3)$$

where n has integer values and is called a quantum number. We'll return to this system a little later in the course and solve the problem of a particle in a three-dimensional box.

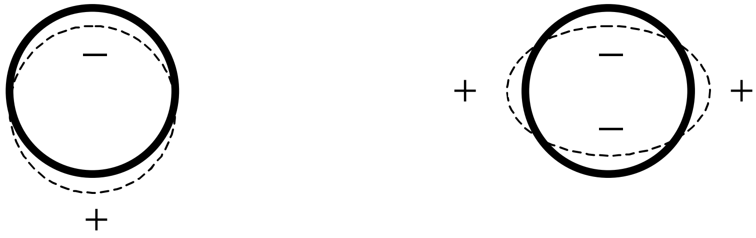
Applied to circular motion of radius R, the condition for a standing wave would read:

$$2\pi R = \lambda n \qquad n = 1, 2, 3... \qquad (4)$$

Comparing Eqs. (3) and (4), we see that the length L of the box has been replaced by the perimeter $2\pi R$ of the circular orbit. Further, the wave must be completely in phase around the orbit, so "half wavelength" states are not permitted in Eq. (4), whereas they are allowed in Eq. (3).

Hydrogen-like atoms

Let's now apply condition (4) to motion governed by a central potential, specifically Coulomb's law. Again, the condition implies that the phase behavior of the de Broglie waves must be something like:



The plus and minus signs are meant to represent spatial regions where the wave has positive or negative values (*i.e.* crests and troughs). Let's combine Eq. (4), the quantization condition, with Eq. (2), the de Broglie wavelength:

$2\pi R = \lambda n$ plus $\lambda = h/p$

yields

$$2\pi R = nh/p$$

or

$$Rp = nh/2\pi.$$

The combination $h/2\pi$ appears sufficiently often that it is given a special symbol $\hbar$, pronounced h-bar. That is,

$$Rp = n\hbar. \qquad (5)$$

Note that the LHS is the classical angular momentum of the particle (we return to this later). This relation between R and p can be used along with Newton's second law to determine the energy of a particle with a particular orbit. To maintain the particle in a circular orbit requires a centripetal force F_{cen} given by

$$F_{\mathrm{cen}} = ma_{\mathrm{cen}} = mv^2/R, \qquad (6)$$

where a_{cen} is the centripetal acceleration given by the usual expression v^2/R. Now, this force arises from the attraction between objects (could be gravitational, even) which, for the hydrogen atom is Coulomb's law

$$F_{\mathrm{coul}} = kQ_1Q_2 / R^2 = kZe^2/R^2. \qquad (7)$$

Here, the charge on the nucleus is Ze and the charge on a single orbiting electron is e, where e has the value 1.6×10^{-19} C. The universal constant $k = 8.99 \times 10^9$ N•m^2/C^2. Now, equate (6) and (7):

$$mv^2/R = kZe^2/R^2,$$

or

$$mv^2 = kZe^2/R. \qquad (8)$$

Using the non-relativistic expression for the momentum $p = mv$, Eq. (5) is

$$v = n\hbar / mR,$$

which can be substituted directly into Eq. (8) to determine R:

$$m\,(n\hbar / mR)^2 = kZe^2/R$$

or

$$R_n = (n\hbar)^2 / mkZe^2 \qquad n = 1, 2, 3, \qquad (9)$$

where we have attached a subscript to R to emphasize that only a discrete set of radii are allowed, corresponding to the standing wave condition. The combination $\hbar^2 / mke^2$ is generally lumped together as the Bohr radius a_o,

$$a_o = \hbar^2 / mke^2 = 0.53\ \text{Å}.$$

In a more compact form, then

$$R_n = n^2 a_o/Z.$$

The energies of the allowed orbits are now easy to determine from the sum of the potential and kinetic energies. Before substituting for specific radii, we recast the total energy E as

$$\begin{aligned} E &= K + V \\ &= mv^2/2 - kZe^2/R. \end{aligned}$$

But from Eq. (8), we see that the kinetic energy has half the magnitude of the potential energy, so we are left with

$$E = -(1/2)\ kZe^2/R. \qquad (10)$$

The minus sign shouldn't bother us, it only indicates that the state is bound. Substituting Eq. (9) into (10) yields

$$E_n = -(m/2)\bullet(kZe^2 / n\hbar)^2. \qquad (11)$$

We'll use these expressions for R_n and E_n later on the in course to discuss the energies and dimensions of atoms. Right now, it is worthwhile pointing out several trends that can be seen from these expressions:

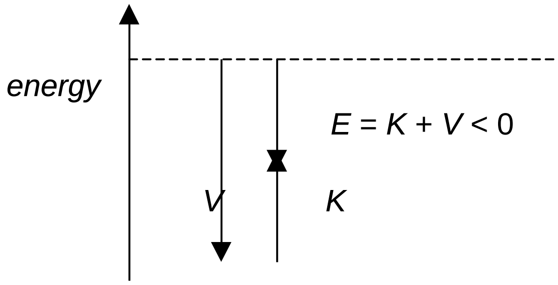
1. For hydrogen-like atoms, meaning one electron orbiting a heavy nucleus,

$R_n \sim 1/Z$	the orbits shrink as Z increases (does not mean *atoms* shrink)
$E_n \sim Z^2$	orbits are more tightly bound as Z increases.

2. Other negative particles than electrons can be bound by a nucleus. Rewrite Eq. (11) a little by introducing the speed of light c:

$$E_n = -mc^2\,(kZe^2 / n\hbar c)^2 / 2.$$

The expression in brackets has not units, and the energy scale is set by mc^2 *of the electron*. If the electron is replaced by a negative *muon*, the energy of the proton-muon system is more deeply bound by a factor of m_μ/m_e, ~ 200 and has a much smaller orbital radius. An energy diagram for this system looks like



Lastly, we return to the quantization condition

$$Rp = n\hbar.$$

For circular orbits, the left hand side is the angular momentum $L = Rp = mvR$. To Bohr, this was the fundamental quantization condition, that angular momentum is quantized according to

$$L = n\hbar.$$

Although we will show that this condition is not quite exact, it is insightful, given that the spin of elementary particles is quantized in units of $\hbar$:

[*spin angular momentum*] ~ $\hbar/2$.