# **Hydrodgen-Deuterium Spectroscopy**

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# 1.0 Atomic physics - a perspective

The idea that matter is made of ultimate particles called atoms goes back to ancient Greek civilization. However, this fundamental view of matter was not completely accepted even by the beginning of the twentieth century. The problem was that there was, until recently, no way to directly verify the existence of such small particles. Now we do have sufficiently good microscopes and are comfortable with the idea that the smallest identifiable piece of any element is indeed the atom. We further understand that atoms themselves are composed of more fundamental particles: protons, neutrons, and electrons. At the atomic scale, the rules of classical physics break down and it is necessary to describe behavior of atomic systems using quantum mechanics.

Atomic and molecular physics aims to understand the internal structure of atoms and how this structure affects the interaction of atoms with their environment, particularly electromagnetic radiation, atomic and electron beams, surrounding atoms, and surfaces. This understanding lays the foundation for several other key areas of physics. For example, chemical physics applies atomic theory to understand the formation and behavior of molecules, while condensed matter physics seeks the connection between the properties of individual atoms and the behavior of atoms aggregated into liquids and solids.

The hydrogen atom is the simplest atom and establishes the foundation for all of the rest of atomic physics. The detailed understanding of the hydrogen atom creates a model for how physics is done, a process that is in many ways distinct from other disciplines such as biology or engineering. Extremely precise experiments are devised to extract quantitative tests of ever more subtle phenomena. Out of this systematic, detailed quantitative study come comprehensive, far-reaching models that apply to much more than atomic hydrogen itself. Thus the simplicity of the system does not imply that the conclusions drawn from its study are trivial or isolated to that system alone. This is a pattern for much of the rest of physics and is a major part of the power and joy of the discipline.

The build-up of larger atoms with more constituent protons, neutrons, and electrons also creates a pattern for physical modeling. In this case, the task is to understand moderately complex systems by separating out dominant interactions and making successive approximations to a basic model. The systematic approach to solving Schrödinger's equations for multi-electron atoms uses such approximation methods and combines them with a fundamental idea called the Pauli exclusion principle to produce a powerfully useful picture of atomic structure. This picture is based on a hierarchy of energy levels or shells that are successively filled as electrons are added to a bare nucleus to create a neutral atom. Even without calculating the details, the idea of the shell structure related to the basic model of the

hydrogen atom successfully explains the remarkable ordering of elemental chemical properties into the system called the periodic table. Nowadays, sophisticated numerical modeling allows us to fill in the details and predict new phenomena and new ways of manipulating atoms.

Much of the behavior of atomic interactions with other atoms can be understood in terms of the most weakly bound electrons: this leads to comprehensive theories of molecules, chemical bonds, adhesion of atoms to surfaces, and even the conformation of complexes of large biological molecules. Meanwhile, deeply-bound electrons can be probed by x-rays or by scattering of very energetic electrons.

Atoms can be manipulated with exquisite delicacy using models of their internal structure and predictions of the responses induced by carefully tuned and timed pulses of light. Thus it is possible to use lasers to cool and trap atoms. It is also possible to observe effects of the quantum interference of atoms viewed as matter waves, and the condensation of a certain class of identical atoms into a single coherent ground state called a Bose condensate.

Optical spectroscopy, the measurement of light as it interacts with matter as a function of wavelength (or energy) of the light, is an extremely important tool in atomic physics. Instruments of great precision, such as diffraction gratings, interferometers, photomultiplier tube detectors, and stabilized lasers, form the tools of the trade. Light levels can vary from the brightness of an intense arc to a few photons per second. Time scales can be as short as femtoseconds and length scales as large as distance across the known universe (where atoms are detected using their characteristic emissions). Wavelengths span ranges from radio (meters) to visible (hundreds of nanometers) to x-rays (nanometers). The precision of atomic and molecular spectroscopy yields several fundamental technologies, such as the atomic clock and the laser.

Another other major type of experiment in atomic and molecular physics uses atomic or molecular beams, and combinations of such beam experiments with electromagnetic probes. Technologies for very high vacuums and ultra-clean surfaces are often involved, and this combination of beams, vacuum systems, optics, etc. has been translated into a wide range of practical technologies for studying and manufacturing advanced technological materials.

The existence of a fundamental quantum mechanical property of atoms and their constituents called spin is the basis for phenomena called magnetic resonance. Magnetic moments associated with these spins give atoms and aggregates of atoms special properties in the presence of magnetic fields. These properties can be manipulated and detected with great precision. The effect of local environments on such properties provides a means to identify chemical compounds and structures called magnetic resonance spectroscopy. The ability to combine clever timing techniques and spatial magnetic field gradients allows these properties to be mapped in three-dimensional space and is the basis for the important medical technology called magnetic resonance imaging.

Finally, tools for the efficient manipulation of individual atoms at the nanometer scale are opening up an area of development called nanotechnology. The exciting prospect exists that useful machines and processes can be custom-designed at the atomic and molecular scale. The impact of such capabilities is expected to be enormous and broad, ranging from information technology to solar energy conversion to biomedicine.

# 1.1 Spectroscopy of hydrogen - an overview

The purpose of this experiment is to relate precise spectroscopic measurements of light from a hydrogen discharge lamp to a heirarchy of more comprehensive models of the structure of atomic hydrogen. The starting point is the Bohr model, developed in 1913 to make a first synthesis of ideas about quantization and the experimental evidence that atoms had dense massive cores (nuclei) surrounded by fast moving electrons.

The Bohr model starts with a classical picture of a negatively-charged electron orbiting a positively-charged nucleaus under the action of a central force, namely Coulomb attraction between oppositely charged particles. We will initially use this semi-classical model for two purposes. The first purpose is to create a readily-derived heuristic for quantifying the overall features of the observed spectrum by explaining the exquisite regularity in the location of the spectral lines. Although we now understand that the Bohr model was overly simplistic and that a full treatment requires quantum mechanics expressed through Schrödinger's equation, this heuristic approach is important for the following reason: it is an example of how one builds bridges of explanation to explain new phenomena using an adroitly chosen mixture of conventional models and critical new assumptions. The hydrogen spectrum itself is now "old news", but new phenomena occur across all the fields of physics whose first exploration requires such bridging models. If you are the first to create such a bridge, you may have the privelege of having the model named after you!

The other use of the Bohr model is to demonstrate how to convert the two-body problem with mutually acting forces into an equivalent single-body problem under a central force. This will introduce the idea of reduced mass and provide the basic quantitative understanding we need to interpret measurements of the shift in spectral lines emitted by the isotope deuterium compared to lines emitted by hydrogen.

As noted above, the Bohr model only goes so far in explaining atomic structure and it was soon replaced by a deeper model based on a complete re-formulation of mechanics at the atomic scale. Schrödinger's equation expressly treats matter in terms of wave-like properties and puts the description of atomic structure (and experimental observations) into a probabilistic framework. Thus electrons are not described by classical orbits but instead occupy states whose mathematical description gives the probability of finding the electron at a given position: often, this is depicted as electron "clouds" in diagrams illustrating the "truer" nature of atoms.

Nonetheless, certain important ideas originating in classical physics carry over into the wavefunction treatment of the hydrogen atom. Chief amongst these are the ideas that electron states can be defined to have definite energy and definite angular momentum. Furthermore, the angular momentum is a vector quantity whose magnitude and direction both must be conserved in the absence of outside perturbations. The consequence of a detailed solution to Schrödinger's equation is that states are labelled by quantum numbers n, l, and  $m_l$  that reflect both the energy and angular momentum of the system. How, in fact, the energy depends on these quantum numbers is a key question that we wish to investigate spectroscopically. The

original Bohr model gives us the dependence on n, the principal quantum number associated with the radial distribution of the electrons. Using Schrödinger's equation, we want to know what connections, if any, also exists between the energy and angular momentum of the system.

In fact, careful experiments show that the information is incomplete for establishing these connections and a fourth quantum number is needed to completely describe the electron state, namely the electron's spin. More precisely, the magnitude s of the spin is fixed for all electrons and it is only the direction specified by the quantum number ms that varies. Associated with spin is a magnetic dipole moment and this magnetic dipole moment interacts with the magnetic field generated by the orbital motion of the same electron. Thus we expect that the energy will depend on how the particular combination of l,  $m_l$ , and  $m_s$  describes the overall angular momentum of the system. Here it will be necessary to introduce yet another quantum number, j, that represents the vector combination of the orbital and spin angular momentum of the electron.

The result of a detailed theoretical analysis shows that there are several effects that jointly contribute to small shifts in energy as the combined angular momentum state is varied. This produces something called a "fine structure" in the observed optical spectra of atomic hydrogen. Thus another goal of this experiment is to assess the feasibility of measuring this fine structure given a detailed understanding of the capabilities of the spectroscopic instrumentation.

Finally, for completeness, it turns out that there is yet another magnetic interaction that the electron experiences. The nucleus (which is just a proton for the simplest isotope of hydrogen) also has spin and an associated magnetic momemnt. Thus there is a magnetic dipole-dipole interaction between the electron and the nucleus, and this produces even smaller changes to the energy state of the system. The resulting "hyperfine" structure will be found to be well outside the capabilities of the instrumentation for this experiment.

# 1.2 The big ideas

When materials are heated or otherwise exposed to external supplies of energy, one possible response is to give off light. A key idea is that this light carries information characteristic of the material from which it is emitted and even of fundamental properties of matter. In this experiment, an electric discharge running through a tube of low-pressure hydrogen creates a glowing mass of gas. The discharge does two things: it dissociates gaseous hydrogen molecules into atoms and it excites the electrons in the atoms to higher energy states. The cascade of electrons from excited states back down to lower states is accompanied by release of energy in the form of photons of light. Thus the light that emerges yields information about the energy states available in hydrogen atoms. The frequencies  $\nu$  of these photons carry information about the change in energy  $\Delta E$  of the cascading electrons according to:

$$\Delta E = h\nu$$
.

Here h is Planck's constant.

In order to extract information from the emitted light, we need some way of dispersing the light into its component frequencies. Notice here that the superposition is at play: we assume that light can propagate as a electromagnetic waves with a mixture of frequencies. The experimental goal is to sort out this mixture into its constituents, that is, to measure the spectrum of the light. To do this, we need a device called a dispersing element. The two most common types of dispersing elements in optical spectroscopy are prisms and diffraction gratings, with the latter serving by far as the most important type in research-grade instruments. Other optical system components, including a light collection lens, entrance and exit slits, mirrors, and a detector are combined with the dispersing element to make a spectrometer. A major goal of this experiment is to understand what determines the resolving power  $\mathbb R$  of a diffraction grating spectrometer. This is defined as:

$$\mathbb{R} = \frac{\lambda}{\Delta \lambda}.$$

where  $\lambda$  is the wavelength of the light being studied and  $\Delta\lambda$  is the smallest separation in wavelength between two spectral components that can still be distinguished.

(A note about notation: below we will use the symbol R to refer to the Rydberg constant, not to be confused with the resolving power  $\mathbb{R}$ .

Note that other possibilities might exist for dividing the light into its spectrum. A detector could be chosen that only responds to specific frequencies: in fact, this is done for radio-frequency and microwave spectroscopy. If the light propagates through a dispersive medium, that is, one in which the speed varies with frequency, one could – at least in principle – sort out pulses of light into constituents based on the time of propagation. In fact, the corresponding spectroscopy for energetic particles emitted from radioactive decays can be measured by so-called time-of-flight spectrometers. Finally, there is a third general method that does indeed play an important role in optical spectroscopy: interferometry. The wavelike nature of light can be exploited by only letting light pass through an instrument if waves of the light constructively interfere: this process is dependent on the wavelength and thus becomes a method for separating different parts of an optical spectrum. We will reconsider the use of interferometric techniques later in this experiment.

It is important to stress that the ideas here based on visible light spectroscopy can and do apply to a whole range of electromagnetic radiation. Thus there are spectroscopic methods for radiofrequency, microwave, infrared, visible, ultraviolet, and x-ray emissions from atomic and molecular sources. It is no accident that the energy transitions that we presently consider for the hydrogen discharge overlap with the portion of the electromagnetic spectrum visible to the human eye: processes in the solar photosphere that produce sunlight largely involve hydrogen and we have evolved to use this sunlight as our means of vision.

When we compare sunlight to the spectrum of the hydrogen discharge lamp, we will observe a major difference: sunlight has a broad continuous spectrum while the discharge spectrum consists of a set of discrete lines. This raises many questions. One key question is: what

processes can broaden the spectrum that would otherwise occur as narrow lines? Two such processes, Doppler broadening and collisional (pressure) broadening, could be subjects for further exploration: see the section "Point of Departure."

# 1.3 Modeling and calculations

In the following sections, you will explore how we constuct models of atomic behavior and, in particular, of the generation of emission spectra. The first is a review of the atomic theory of hydrogen, starting with the Bohr model, introducing the idea of reduced mass, and progressing to a summary of solutions of the Schrödinger equation. A goal is to predict energies of transition between states defined by an appropriate set of quantum numbers. We will see how the effect of reduced mass and the instrumental ability to distinguish between the spectra of hydrogen and deuterium will allow us to determine a fundamental property of nature: the ratio of the mass of the electron to the mass of the proton.

### 1.4 The Bohr model and atomic scales

## 1.4.1 Equations in non-dimensional form

We will first approach the semi-classical Bohr model with very general ideas about dynamics and dimensional analysis. We start by assuming that the nucleus is so much more massive than the electron that we can model the system as a electron with negative charge -e and mass m orbiting an infinitely massive charge +e of the same magnitute located at the origin. The electron state is then described by its position  $\mathbf{r}$  relative to the nucleus and its momentum  $\mathbf{p}$ , both of which vary with time t. A Coulomb force acts on the electron of form:

$$\mathbf{F} = -\frac{e^2}{4\pi\epsilon_0 r^2} \hat{\mathbf{r}}.$$

Show that the dynamics of the problem can be written down as the coupled system of equations:

$$\frac{d\mathbf{r}}{dt} = \frac{1}{m}\mathbf{p}.$$

$$\frac{d\mathbf{p}}{dt} = -\frac{e^2}{4\pi\epsilon_0 r^2}\hat{\mathbf{r}}.$$

#### **ANSWER**

By definition of momentum  $\mathbf{p} = m\mathbf{v}$  and definition of velocity  $\mathbf{v} = \frac{d\mathbf{r}}{dt}$ , we have the first relation

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} = \frac{1}{m}\mathbf{p}.$$

By Newton's Second Law in momentum form:

$$\frac{d\mathbf{p}}{dt} = \mathbf{F},$$

so substituting the Coulomb expression for the electrostatic force

$$\frac{d\mathbf{p}}{dt} = -\frac{e^2}{4\pi\epsilon_0 r^2}\hat{\mathbf{r}}.$$

In a manner similar to that used in the mechanics and the thermodynamics experiments, we want to find a way to express the dynamics of the problem in "natural scales" of the system. Somehow we want to derive such natural scales out of the fundamental constants of the problem. So far, these fundamental constants include the electron mass m, the magnitude of the electron charge e, and the permittivity of free space e0. Are these sufficient to define the typical size for atoms?

#### **EXCERCISE 2**

Suppose the radial position of the electron has typical scale  $r_0$ , the momentum has typical scale  $p_0$ , and the time for significant change in the position and momentum has typical scale  $t_0$ . Use the equations from exercise 1 to write down two relations between these three scales.

Let the atomic number be Z = 1.

Hint: let

$$r = r_0 r',$$

$$p = p_0 p',$$

$$t = t_0 t'.$$

where r', p', and t' are dimensionless. For the equations of motion, collect all of the dimensioned terms onto the right-hand side into single groups which then must dimensionless. Set each group equal to unity to achieve a "natural" scale. This sets up two relationships with the three unknown scales  $r_0$ ,  $p_0$ , and  $t_0$ .

#### **ANSWER**

Do the change of variables in the equations of motion:

$$\frac{r_0}{t_0} \frac{d\mathbf{r'}}{dt'} = \frac{1}{m} p_0 \mathbf{p'}.$$

$$\frac{p_0}{t_0} \frac{d\mathbf{p'}}{dt'} = -\frac{1}{r_0^2} \frac{e^2}{4\pi\epsilon_0 r'^2} \hat{\mathbf{r}}.$$

Group the dimensioned terms on the right:

$$\frac{d\mathbf{r}'}{dt'} = \frac{t_0}{m} \frac{p_0}{r_0} \mathbf{p}'.$$

$$\frac{d\mathbf{p}'}{dt'} = -\frac{e^2}{4\pi\epsilon_0} \frac{t_0}{p_0 r_0^2} \frac{\hat{\mathbf{r}}}{r'^2}.$$

Set the scale groupings equal to unity since the groupings must be dimensionless:

$$\frac{\frac{t_0}{m} \frac{p_0}{r_0}}{\frac{e^2}{4\pi\epsilon_0} \frac{t_0}{p_0 r_0^2}} = 1.$$

Then in natural sales the dynamics becomes

$$\frac{d\mathbf{r}'}{dt'} = \mathbf{p}'.$$

$$\frac{d\mathbf{p}'}{dt'} = -\frac{\hat{\mathbf{r}}}{r'^2}.$$

Let's rearrange our scale relationships to get:

$$\frac{p_0 t_0}{r_0} = m.$$

$$\frac{t_0}{p_0 r_0^2} = \frac{4\pi\epsilon_0}{e^2}.$$

# 1.4.2 Introducing Planck's constant by postulating a third relation between scales

So far we have only two equations, which are insufficient to determine the three unknown scales. And yet we know that atoms have a definite size, so this suggests that there must be an additional piece of physics involved. Here is where quantum theory introduces a completely new idea. We will postulate that the position and momentum scales are related by:

$$r_0 p_0 = \hbar$$
.

where  $\hbar$  is Planck's constant h divided by  $2\pi$ .

There are several interpretations of this postulate. One, following ideas introduced by Bohr, is that the angular momentum  $L=r\times p$  of the system is quantized in steps of size  $\hbar$ . Another interpretation is that the postulate expresses the uncertainty principle: the product of the position and momentum scales must be fixed so that we cannot know both to arbitrary position. Whatever the interpretation, we now have three relations in three unknowns and a surprizing amount can be learned about the hydrogen atom just from this reasoning.

# 1.4.3 Finding the atomic length, time, and momentum scales

#### **EXERCISE 3**

(a) Use the postulated position-momentum relation and the results of exercise 2 to show that the length scale can be written as

$$r_0 = a_0$$

where  $a_0$  denotes the "Bohr radius" given by:

$$a_0 \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2}.$$

- (b) Now find an expression for the natural time scale  $t_0$ .
- (c) Finally find an expression for the natural momentum scale  $p_0$ .

#### **ANSWER**

(a) We have the three relations

$$\frac{p_0 t_0}{r_0} = m.$$

$$\frac{t_0}{p_0 r_0^2} = \frac{4\pi\epsilon_0}{e^2}.$$

$$r_0 p_0 = \hbar.$$

Use the second equation to isolate t\_0:

$$t_0 = \frac{4\pi\epsilon_0}{e^2} p_0 r_0^2.$$

Put this into the first equation:

$$\frac{4\pi\epsilon_0}{e^2}\frac{p_0^2r_0^2}{r_0}=m.$$

Now use the third relation  $r_0p_0=\hbar$  in the numerator of the above equation:

$$\frac{4\pi\epsilon_0}{e^2}\frac{\hbar^2}{r_0}=m.$$

Solve for  $r_0$ :

$$r_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} \equiv a_0.$$

(b) For the time scale

$$t_0 = \frac{mr_0}{p_0} = \frac{mr_0^2}{\hbar} = \frac{m}{\hbar} \left(\frac{4\pi\epsilon_0\hbar^2}{me^2}\right)^2$$

So

$$t_0 = \frac{(4\pi\epsilon_0)^2\hbar^3}{me^4}.$$

(c) Substitute for  $\emph{r}_0$  in the equation

$$p_0 = \frac{\hbar}{r_0}$$

to get

$$p_0 = \frac{me^2}{4\pi\epsilon_0\hbar}.$$

# 1.4.4 Atomic scale for velocity

#### **EXERCISE 4**

Writing a velocity scale as  $v_0=rac{p_0}{m}$ , find an expression for the relativistic factor  $eta_0\equivrac{v_0}{c}$ .

#### **ANSWER**

The velocity scale

$$v_0 = \frac{p_0}{m} = \frac{1}{m} \frac{me^2}{4\pi\epsilon_0 \hbar},$$

so

$$v_0 = \frac{e^2}{4\pi\epsilon_0 \hbar}$$

and

$$\frac{v_0}{c} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar c}.$$

# 1.4.5 Atomic scale for energy

#### **EXERCISE 5**

(a) What combination of  $r_0$ ,  $p_0$  and  $t_0$  has units of energy? Use this combination to show that there is a natural energy scale  $E_0$  given by

$$E_0 \equiv \frac{me^4}{(4\pi\epsilon_0)^2\hbar^2}.$$

(b) Also show that this energy scale is equal to the magnitude of the electrostatic potential energy |V(r)| evaluated at the Bohr radius  $a_0$ :

$$E_0 = \frac{e^2}{4\pi\epsilon_0 a_0}.$$

This unit of energy is called the *Hartree* and will be found below to be twice the absolute value of the ground state energy of hydrogen.

#### **ANSWER**

(a) The following combination has units of energy since  $p_0/t_0$  has units of force and  $r_0$  has units of distance so their product has units of work, i.e. energy:

$$E_0 = \frac{p_0}{t_0} r_0.$$

Evaluating the energy scale:

$$E_0 = \frac{p_0}{t_0} r_0 = \frac{\frac{me^2}{4\pi\epsilon_0\hbar}}{\frac{(4\pi\epsilon_0)^2\hbar^3}{me^4}} \frac{4\pi\epsilon_0\hbar^2}{me^2} = \frac{me^4}{(4\pi\epsilon_0)^2\hbar^2}.$$

Summarizing:

$$E_0 = \frac{me^4}{(4\pi\epsilon_0)^2\hbar^2}.$$

(b) Using

$$a_0 \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2}$$

so that

$$\frac{1}{a_0} = \frac{me^2}{4\pi\epsilon_0\hbar^2},$$

we see that

$$\frac{e^2}{4\pi\epsilon_0} \frac{1}{a_0} = \frac{e^2}{4\pi\epsilon_0} \frac{me^2}{4\pi\epsilon_0 \hbar^2} = \frac{me^4}{(4\pi\epsilon_0)^2 \hbar^2} = E_0.$$

So indeed

$$E_0 = \frac{e^2}{4\pi\epsilon_0 a_0}.$$

## 1.4.7 Relationship between energy and time scales

**EXERCISE 6** 

What is the product  $E_0 t_0$  of the energy and time scales?

**ANSWER** 

$$E_0 t_0 = \frac{me^4}{(4\pi\epsilon_0)^2\hbar^2} \frac{(4\pi\epsilon_0)^2\hbar^3}{me^4}.$$
 $E_0 t_0 = \hbar$ 

which is another reflection of uncertainty relations.

#### 1.4.8 Numerical values of the atomic scales

Now it would be good to find numerical values for these scales. You could look up all of the constants in a handbook, but it is strongly recommended that you memorize the following four relations. These will be very useful for back-of-the-envelope calculations for physics at the atomic scale.

The energy equivalent of the rest mass of the electron is:

$$mc^2 = 0.511 \times 10^6 \text{ eV}.$$

A useful combination for later calculating photon energy is:

$$hc = 1240 \text{ eV nm}$$
.

A very important dimensionless number called the fine-structure constant gives us a way of scaling electric charge interaction:

$$\alpha \equiv \sqrt{\frac{E_0}{mc^2}} = \sqrt{\frac{\frac{e^2}{4\pi\epsilon_0 a_0}}{mc^2}} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar c} = \frac{1}{2\epsilon_0} \frac{e^2}{\hbar c} = \frac{1}{137}.$$

See: <a href="https://en.wikipedia.org/wiki/Fine-structure\_constant">https://en.wikipedia.org/wiki/Fine-structure\_constant</a> (https://en.wikipedia.org/wiki/Fine-structure\_constant)

Finally we have the speed of light:

$$c = 3.00 \times 10^8 \text{ ms}^{-1} = 3.00 \times 10^{17} \text{ nm s}^{-1}$$
.

Using these quantities, find values for the

- (a) Bohr radius  $a_0$  in nanometers,
- (b) the Hartree  $E_0$  in electron volts, and
- (c) the electron velocity scale divided by the speed of light  $\frac{v_0}{c}$  (hint: relate this to the fine structure constant).

#### **ANSWER**

(a) 
$$a_0 \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2} = \frac{4\pi\epsilon_0\hbar c}{e^2} \frac{hc}{2\pi mc^2} = \frac{1}{\alpha} \frac{hc}{2\pi mc^2} = 137 \frac{1240 \text{ eV nm}}{2\pi \times 0.511 \times 10^6 \text{eV}} = 0.0529 \text{ nn}$$

(b) 
$$E_0 = \frac{me^4}{(4\pi\epsilon_0)^2\hbar^2} = mc^2 \frac{e^4}{(4\pi\epsilon_0)^2\hbar^2c^2} = \alpha^2 mc^2 = \frac{1}{137^2} 0.511 \times 10^6 \text{ eV} = 27.2 \text{ eV}$$

(c) 
$$\frac{v_0}{c} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar c} = \alpha = \frac{1}{137}.$$

For completeness, use the same useful quantities to find

- (a) the time scale  $t_0$
- (b) the momentum scale  $p_0$ : express this as the product  $p_0c$ .

#### **ANSWER**

(a) Time scale

$$t_0 = \frac{(4\pi\epsilon_0)^2\hbar^3}{me^4}.$$

$$t_0 = \frac{(4\pi\epsilon_0)^2\hbar^2c^2}{e^4}\frac{hc}{2\pi}\frac{1}{mc^2}\frac{1}{c} = \frac{1}{2\pi}\frac{1}{\alpha^2}hc\frac{1}{mc^2}\frac{1}{c}.$$

$$t_0 = \frac{1}{2\pi} 137^2 1240 \text{ eV nm } \frac{1}{0.511 \times 10^6 \text{eV}} \frac{1}{3.00 \times 10^{17} \text{ nm s}^{-1}} = 2.42 \times 10^{-17} \text{ s} = 0.$$

(b) Momentum scale

$$p_0 = \frac{me^2}{4\pi\epsilon_0 \hbar}.$$
 
$$p_0 c = \frac{e^2}{4\pi\epsilon_0 \hbar c} mc^2 = \alpha mc^2 = \frac{1}{137} 0.511 \times 10^6 \text{ eV} = 3730 \text{ eV}.$$

# 1.5 Energy levels of the hydrogen atom

Now that we have established scales for the hydrodgen atom, we should try to find the actual energy states of the electron. It is, after all, transitions between these energy states that are responsible for the light given off by the hydrogen discharge lamp.

We could proceed to find solutions to the dynamical equations in dimensionless form, but at this point it is more instructive to return to the Bohr model with dimensions included. In this model, the electron is assumed to move in a circular orbit and thus is constantly accelerating. According to classical electrodynamics, an accelerating charged particle should radiate electromagnetic waves and thus continuously lose energy. This predicts that the orbiting electron should spiral into the nucleus. Bohr sought a model that would only allow the electron to occupy certain orbits separated by finite steps in energy. Continuous radiation would be forbidden because a continuum of intermediate orbits would not be available. Moreover, there would be a smallest ground state orbit from which no further energy loss would be possible.

(Note: a similar argument can be used to explain superfluidity: resistance to fluid motion requires momentum exchange, but for a quantum fluid with small enough velocity through a channel, states are not available to exchange momentum with the walls.)

#### **EXERCISE 9**

Write down Newton's Second Law for circular motion of an electron of mass m and charge -e about an infinitely massive nucleus of charge +e.

#### **ANSWER**

Identifying the centripetal acceleration as  $-v^2/r$ , we have from Newton's 2nd Law (assuming circular orbits):

$$-m\frac{v^2}{r} = -\frac{e^2}{4\pi\epsilon_0 r^2}.$$

How is the kinetic energy K and the total energy E related to the potential energy V(r)?

#### **ANSWER**

So from above, the kinetic energy K can be related to the potential energy V(r) as

$$K = \frac{1}{2}mv^2 = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0 r} = -\frac{1}{2}V(r).$$

The total energy E = K + V(r) is then

$$E = -\frac{1}{2}V(r) + V(r) = \frac{1}{2}V(r) = -\frac{1}{2}\frac{e^2}{4\pi\epsilon_0 r}.$$

Bohr provided a rule for selecting allowed orbits equivalent to stating that the angular momentum is quantized. However, we will jump ahead to a wave-mechanics interpretation of the quantization by employing de Broglie's hypothesis that the electron has wavelike properties. The wavelength is related to the momentum by:

$$\lambda = \frac{h}{p} = \frac{h}{mv}.$$

The allowable orbits will be those for which the electron orbit accommodates a standing wave. The circumference of the orbit must consist of an integer number of wavelengths:

$$2\pi r = n\lambda$$
.

Show that this requirement on the wavelength and the de Broglie relation lead to quantization of the orbital angular momentum:

$$L = mvr = n\hbar$$
,

**ANSWER** 

$$L = mvr = mv\frac{n\lambda}{2\pi} = mv\frac{1}{2\pi}n\frac{h}{mv} = n\frac{h}{2\pi} = n\hbar.$$

The quantization condition now provides an additional relation connecting the radius to the kinetic energy.

Combine the quantization of angular momentum with the expression for Newton's Law in Exercise 5 to show that the radius and energy of an orbit specified by quantum number n is given by:

$$r_n = a_0 n^2$$
.

$$E_n=-\frac{E_0}{2}\frac{1}{n^2}.$$

where  $a_0$  and  $E_0$  are given in Exercises 3 and 4 and the total energy is related to the potential energy in Exercise 6.

#### **ANSWER**

From Newton's 2nd Law:

$$-m\frac{v^2}{r} = -\frac{e^2}{4\pi\epsilon_0 r^2}.$$

we have

$$(mvr)^2 = m\left(m\frac{v^2}{r}\right)r^3 = m\frac{e^2}{4\pi\epsilon_0 r^2}r^3 = \frac{me^2}{4\pi\epsilon_0}r.$$

Then quantization of angular momentum gives:

$$n^2\hbar^2 = \frac{me^2}{4\pi\epsilon_0}r.$$

So

$$r = n^2 \frac{4\pi\epsilon_0 \hbar^2}{me^2} = n^2 a_0.$$

Now using the fact from Exercise 6 that

$$E = -\frac{e^2}{4\pi\epsilon_0 r}$$

we have

$$E = -\frac{1}{2} \frac{e^2}{4\pi\epsilon_0 n^2 a_0} = -\frac{1}{n^2} \frac{1}{2} \frac{e^2}{4\pi\epsilon_0 a_0} = -\frac{1}{n^2} \frac{E_0}{2}.$$

# 1.6 Wavelengths of light emitted by excited hydrogen atoms

If an electron makes a transition from an *initial* excited state  $n_i$  to a *final* lower state  $n_f$ , it loses energy  $\Delta E = E_i - E_f$ . Energy conservation is satisfied if the transition is accompanied by emission of a photon. The photon's wavelength is related to its energy by

$$\Delta E = \frac{hc}{\lambda}.$$

(a) Show that the wavelength the photon emitted due to a transition from state to is given by:

$$\frac{1}{\lambda} = R_{\infty} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right).$$

where  $R_{\infty}$  is a suitable combination of constants  $m, e, \epsilon_0$ , and h.

Note: Here  $R_{\infty}$  is called the Rydberg constant for an infinitely massive nucleus.

(b) What is the numerical value for  $R_{\infty}$  in  $m^{-1}$  ? (Use the groupings  $hc,mc^2$ , and  $\alpha$  to calculate this.)

#### **ANSWER**

(a)

$$\frac{1}{\lambda} = \frac{\Delta E}{hc} = \frac{1}{hc}(E_i - E_f) = \frac{1}{hc} \left[ -\frac{1}{n_i^2} \frac{E_0}{2} - \left( -\frac{1}{n_f^2} \frac{E_0}{2} \right) \right] = \frac{1}{hc} \frac{E_0}{2} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right).$$

We see that the Rydberg constant is given by

$$R_{\infty} = \frac{1}{hc} \frac{E_0}{2} = \frac{1}{hc} \frac{1}{2} \frac{me^4}{(4\pi\epsilon_0)^2 \hbar^2} = \frac{me^4}{8\epsilon_0^2 h^3 c}.$$

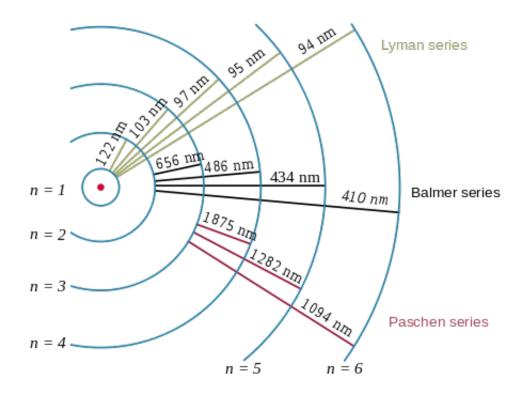
(b) Previously (Exercise 5b) we had

$$E_0 = \alpha^2 mc^2,$$

SO

$$R_{\infty} = \frac{1}{hc} \frac{E_0}{2} = \frac{1}{2} \frac{1}{hc} \alpha^2 mc^2 = \frac{1}{2} \frac{1}{1240 \text{ eV nm}} \frac{1}{137^2} 0.511 \times 10^6 \text{ eV} = 0.01097 \text{ nm}^{-1}$$

The wavelengths emitted in the visible region all correspond to the series where  $n_f = 2$  and  $n_i = 3, 4, 5, ...$  This is called the Balmer series. The red line at 656.3 nm for  $n_i = 3$  transitioning to  $n_f = 2$  is called the *hydrogen alpha line*. (Subsequent lines for 3, 4, 5,... are then beta, gamma, delta,...)



(https://commons.wikimedia.org/wiki/File:Hydrogen\_transitions.svg)

https://commons.wikimedia.org/wiki/File:Hydrogen\_transitions.svg (https://commons.wikimedia.org/wiki/File:Hydrogen\_transitions.svg)

# 1.7 Center-of-mass coordinates and reduced mass

Now we must correct for the fact that the nucleus is not infinitely massive. Thus we start by writing the dynamics for both the electron of mass m acted upon by force FNe ("nucleus-on-electron") and the nucleus of mass M acted upon by force FeN ("electron-on-nucleus"):

$$m\frac{d^2\mathbf{r}_e}{dt^2}=\mathbf{F}_{Ne}.$$

$$M\frac{d^2\mathbf{r}_N}{dt^2}=\mathbf{F}_{eN}.$$

Show that by subtracting a suitable multiple of the second equation from a suitable multiple of the first equation, and using Newton's Third Law that  $\mathbf{F}_{eN} = -\mathbf{F}_{Ne}$ , one can get the following equation for the second derivative of the relative position vector  $\mathbf{r} = \mathbf{r}_e - \mathbf{r}_N$ :

$$\frac{Mm}{m+M}\frac{d^2\mathbf{r}}{dt^2}=\mathbf{F}_{Ne}.$$

#### **ANSWER**

Multiply the first equation by M and subtract the second equation multiplied by m:

$$Mm\frac{d^2\mathbf{r}_e}{dt^2} - mM\frac{d^2\mathbf{r}_N}{dt^2} = M\mathbf{F}_{Ne} - m\mathbf{F}_{eN}.$$

Grouping terms on the left and use  $\mathbf{F}_{eN} = -\mathbf{F}_{Ne}$  ,

$$Mm\frac{d^2(\mathbf{r}_e - \mathbf{r}_N)}{dt^2} = M\mathbf{F}_{Ne} - m(-\mathbf{F}_{Ne}).$$

Thus

$$\frac{Mm}{M+m}\frac{d^2(\mathbf{r}_e-\mathbf{r}_N)}{dt^2}=\mathbf{F}_{Ne}$$

or, defining  $\mathbf{r} \equiv \mathbf{r}_e - \mathbf{r}_N$ ,

$$\frac{Mm}{M+m}\frac{d^2\mathbf{r}}{dt^2} = -\frac{e^2}{4\pi\epsilon_0 r^2}\hat{\mathbf{r}}.$$

We define the reduced mass  $\mu$  by

$$\mu \equiv \frac{Mm}{M+m} = \frac{1}{1+\frac{m}{M}}m.$$

Recalling that the force of the nucleus on the electron  $\mathbf{F}_{Ne}$  is just the Coulomb force, we write the dynamics as:

$$\mu \frac{d^2 \mathbf{r}}{dt^2} = -\frac{e^2}{4\pi\epsilon_0 r^2} \hat{\mathbf{r}}.$$

Thus all of the results from section for the Bohr model must be corrected by replacing the mass m of the electron with the reduced mass  $\mu$ . Most importantly, the energy states are given by:

$$E_n = -\frac{1}{2} \frac{\mu e^4}{(4\pi\epsilon_0)^2 \hbar^2} = -\frac{1}{2} \frac{\mu}{m} \frac{m e^4}{(4\pi\epsilon_0)^2 \hbar^2} = -\frac{\mu}{m} \frac{E_0}{2} \frac{1}{n^2}.$$

where again

$$E_0 \equiv \frac{me^4}{(4\pi\epsilon_0)^2\hbar^2}.$$

#### **EXERCISE 15**

Show that the reduced mass of the electron is approximately:

$$\mu \approx \left(1 - \frac{m}{M}\right) m.$$

**ANSWER** 

$$\mu \equiv \frac{Mm}{M+m} = \frac{1}{1+\frac{m}{M}}m \approx \left(1-\frac{m}{M}\right)m \text{ for } m << M.$$

# 1.8 Application to hydrogen-deuterium spectra

## 1.8.1 Rydberg values

Now the actual wavlength  $\lambda$  for transitions from states  $n_i$  and  $n_f$  is given by:

$$\frac{1}{\lambda} = \frac{\mu}{m} R_{\infty} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right).$$

In calculating the reduced masses for hydrogen and deuterium, we will replace M avove with nuclear masses denoted by  $M_p$  (proton mass) and  $M_{D+}$  (deuteron mass) respectively.

See the appendix for the masses of the hydrogen (H) nucleus (a proton) and the deuterium (D) nucleus. Use these to calculate values for the appropriate Rydberg constants  $R_H$  and  $R_D$  defined by multiplying  $R_\infty$  by the appropriate correction factor. For completeness, include  $R_\infty$  in your list. Express the results in  ${\rm cm}^{-1}$ .

#### **ANSWER**

Reduced mass ratios

$$\frac{\mu_D}{m} = \frac{1}{1 + \frac{m_e}{M_{D^+}}} = 0.999728.$$

$$\frac{\mu_H}{m} = \frac{1}{1 + \frac{m_e}{M_p}} = 0.999457.$$

Calculating more precisely (see the appendix for the more precise values of hc,  $mc^2$ , and  $\alpha$ :

$$R_{\infty} = \frac{1}{hc} \frac{E_0}{2} = \frac{1}{2} \frac{1}{hc} \alpha^2 mc^2 = \frac{1}{2} \frac{1}{1239.86 \text{ eV nm}} \frac{1}{137.036^2} 0.510999 \times 10^6 \text{ eV} = 0.0$$

The published value is actually (to this precision)  $1.09737 \times 10^7 \ m^{-1}$ . (see ), so we will use this published value instead.

Then

$$R_D = 0.999728 \times 1.09737 \times 10^7 \text{ m}^{-1} = 1.09707 \times 10^7 \text{ m}^{-1}.$$

$$R_H = 0.999457 \times 1.09737 \times 10^7 \text{ m}^{-1} = 1.09677 \times 10^7 \text{ m}^{-1}.$$

# 1.8.2 Wavelength shifts and proton-to-electron mass ratio

#### **EXERCISE 17**

Let  $\lambda_H$  be the wavelength of a hydrogen line and let  $\lambda_D$  be the wavelength of the same line for deuterium. Also let  $M_H$  be the nuclear mass of hydrodgen and  $M_D$  the nuclear mass of deuterium. Show that, to lowest order in  $\frac{m}{M_p}$ , the shift in wavelength going from one isotope to the other is:

$$rac{\lambda_H - \lambda_D}{\lambda_H} pprox rac{m}{M_p} \left( 1 - rac{M_p}{M_{D^+}} 
ight).$$

Compute the value of the right-hand side.

**ANSWER** 

$$\frac{\frac{1}{\lambda_D} - \frac{1}{\lambda_H}}{\frac{1}{\lambda_D}} = \frac{\left(\frac{\mu_D}{m} - \frac{\mu_H}{m}\right)}{\frac{\mu_D}{m}} \frac{R_{\infty} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)}{R_{\infty} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)}.$$

$$\lambda_D \left(\frac{1}{\lambda_D} - \frac{1}{\lambda_H}\right) = 1 - \frac{\mu_H}{\mu_D}.$$

$$\lambda_D \frac{\lambda_H - \lambda_D}{\lambda_H \lambda_D} = 1 - \frac{\frac{1}{1 + \frac{m}{M_D}}}{\frac{1}{1 + \frac{m}{M_D^+}}}.$$

$$\frac{\lambda_H - \lambda_D}{\lambda_H} = 1 - \frac{1 + \frac{m}{M_D^+}}{1 + \frac{m}{M_p}}.$$

$$\frac{\lambda_H - \lambda_D}{\lambda_H} \approx 1 - \left(1 + \frac{m}{M_D^+}\right) \left(1 - \frac{m}{M_p}\right).$$

$$\frac{\lambda_H - \lambda_D}{\lambda_H} \approx \frac{m}{M_p} - \frac{m}{M_{D^+}}.$$

$$\frac{\lambda_H - \lambda_D}{\lambda_H} \approx \frac{m}{M_p} \left(1 - \frac{M_p}{M_D^+}\right).$$

Now we compute the value of the right-hand side assuming the proton-to-electron mass ratio is known:

$$\frac{\lambda_H - \lambda_D}{\lambda_H} \approx \frac{m}{M_p} \left( 1 - \frac{M_p}{M_{D^+}} \right) = 0.0005446170215 * \left( 1 - \frac{1}{1.999} \right) = 0.0002722.$$

So

$$\lambda_H - \lambda_D = 0.0002722 \ \lambda_H.$$

Notice that we can reverse this to obtain the ratio of proton mass to electron mass from each spectral line and its isotope shift:

$$\frac{M_p}{m} \approx \left(1 - \frac{M_p}{M_{D^+}}\right) \frac{\lambda_H}{\lambda_H - \lambda_D} = 0.4997 \frac{\lambda_H}{\lambda_H - \lambda_D}.$$

## 1.8.3 Required resolving power

#### **EXERCISE 18**

The resolving power of a spectrometer is defined to be the wavelength  $\lambda$  of a line divided by the separation in wavelength  $\Delta\lambda$  to the closest distinguishable line:

$$\mathbb{R} \equiv \frac{\lambda}{\Delta \lambda}.$$

Rounded to the nearest hundred, what numerical resolving power must a spectrometer have to detect the hydrogen - deuterium line shift?

#### **ANSWER**

We see from the previous exercise that the minimum required resolving power is to lowest order independent of wavelength

$$\mathbb{R}_{\min} = \frac{\lambda_H}{\lambda_H - \lambda_D} \approx \frac{M_p}{m} \frac{1}{1 - \frac{M_p}{M_{D^+}}} = 1836.15 \frac{1}{1 - \frac{1}{1.999}} = 3674.$$

# 1.8.4 Table of wavelengths, wavelength shifts, and ionization energies

#### **EXERCISE 19**

Write python code or create a spreadsheet to provide the first ten wavelengths of the Balmer series calculated for infinitely massive nucleus, hydrogen nucleus, and deuterium nucleus. In the first column, list the values of ni. In the last row, show the limiting wavelength of the series as  $n_i \to \infty$ . In the last column show the difference in wavelengths between hydrogen and deuterium. Include enough precision to express this difference to two significant digits.

```
In [35]: # ANSWER
        Rinf = 0.0109737 \# nm-1
        RD4 = 0.0109707 \# nm-1
        RH5 = 0.0109677 \# nm-1
        print('Wavelengths')
        print(' Infinite
                           Deuterium Hydrogen
                                                     Differrence
                                                                   ApproxDiff
                                                                                (nm
        for n in range(3,13):
         wavelengthinf = 1/(Rinf*(1/4 - 1/n**2))
         12 wavelengthD = 1/(RD*(1/4 - 1/n**2))
         13 wavelengthH = 1/(RH*(1/4 - 1/n**2))
         14 wdifference = wavelengthH - wavelengthD
         adifference = 0.0002722*wavelengthH
         16 print('{0: 10.4f} {1: 10.4f} {2: 10.4f} {3: 10.4f} {4: 13.4f}'.format
        print()
        print('Ionization wavelength (nm)')
        wavelengthinf = 4/Rinf
        wavelengthD = 4/RD
        wavelengthH = 4/RH
        wdifference = wavelengthH - wavelengthD
        adifference = 0.0002722*wavelengthH
        print('{0: 10.4f} {1: 10.4f} {2: 10.4f} {3: 10.4f} {4: 13.4f}'.format(way
        print()
        hc9= 1239.856346
        print('Ionization energy (eV)')
        print('{0: 10.6f} {1: 10.6f} {2: 10.6f} {3: 10.6f}'.format(hc/wavelength
         Wavelengths
           Infinite
                                               Differrence
                      Deuterium Hydrogen
                                                             ApproxDiff
                                                                         (nm)
           656.1142
                      656.2936
                                 656.4731
                                               0.1795
                                                             0.1787
           486.0105
                      486.1434
                                 486.2764
                                               0.1330
                                                             0.1324
           433.9379
                      434.0566
                                 434.1753
                                               0.1187
                                                             0.1182
           410.0714
                      410.1835
                                 410.2957
                                               0.1122
                                                             0.1117
                                              0.1086
           396.9086
                      397.0171
                                 397.1257
                                                             0.1081
           388.8084
                      388.9147
                                 389.0211
                                               0.1064
                                                             0.1059
           383.4433
                      383.5482
                                 383.6531
                                               0.1049
                                                             0.1044
           379.6957
                      379.7995
                                 379.9034
                                               0.1039
                                                             0.1034
           376.9697
                      377.0728
                                 377.1759
                                               0.1031
                                                             0.1027
           374.9224
                      375.0249
                                 375.1275
                                               0.1026
                                                             0.1021
         Ionization wavelength (nm)
           364.5079
                                 364.7073
                      364.6075
                                               0.0997
                                                             0.0993
         Ionization energy (eV)
           3.401453
                      3.400523
                                              0.000930
                                 3.399593
```

# 1.9 Obtaining the ratio of electron mass to proton mass from the ratio of Rydberg constants for deuterium and hydrogen

When we plot  $1/\lambda$  versus  $1/n_i^2$  we get

slope = 
$$R_M = \frac{\mu}{m} R_{\infty} = \frac{1}{1 + \frac{m}{M}} R_{\infty}$$
.

#### **EXERCISE 20**

Show that the ratio of electron mass to proton mass (to a first order approximation in this ratio) is related to the ratio of the slopes, that is, the ratio of the Rydberg constants for each type of atom:

$$\frac{m}{M_p} pprox rac{rac{R_D}{R_H} - 1}{1 - rac{M_p}{M_{D^+}}}.$$

#### **ANSWER**

The ratio of the slopes is

$$\frac{R_D}{R_H} = \frac{\frac{\mu_D}{m} R_{\infty}}{\frac{\mu_H}{m} R_{\infty}} = \frac{\frac{1}{1 + \frac{m}{M_D^+}} R_{\infty}}{\frac{1}{1 + \frac{m}{M_D}} R_{\infty}} = \frac{1 + \frac{m}{M_D}}{1 + \frac{m}{M_D^+}} \approx \left(1 + \frac{m}{M_D}\right) \left(1 - \frac{m}{M_D^+}\right) = 1 + m\left(\frac{m}{M_D^+}\right)$$

Rearranging:

$$rac{m}{M_p}pproxrac{rac{R_D}{R_H}-1}{1-rac{M_p}{M_{D^+}}}.$$

To the level of approximation we are using (see data below),

$$\frac{M_D}{M_H} = 1.999$$

so

$$\frac{m}{M_p} \approx \frac{\frac{R_D}{R_H} - 1}{1 - \frac{1}{1.999}} = 2.001 \left(\frac{R_D}{R_H} - 1\right).$$

It is more common perhaps to see the reciprocal

$$\frac{M_p}{m} \approx \frac{0.4997}{\frac{R_D}{R_H} - 1}.$$

In the experiment, you will use your data find the ratio of slopes as a measure of  $\frac{R_D}{R_H}$ .

#### **EXERCISE 21**

Compute the value of the above expression for the ratio of proton mass to electron using the answers to exericse 12 for the Rydbergs. Compare it to the accepted value (see appendix) = 1836.

**ANSWER** 

$$\frac{m}{M_p} \approx 2.001 \left(\frac{R_D}{R_H} - 1\right) = 2.001 \left(\frac{1.09707}{1.09677} - 1\right) = 2.001 \times .0002735 = 0.0005473$$

$$\frac{M_p}{m} \approx 1/.0005473 = 1827.$$

This is within 0.5% of the published value of 1836.

# 1.10 Point of departure - intrinsic sources of spectral line broadening

The above discussion hinges on the expectation that the spectral lines of hydrogen and deuterium can be distinguiesed from one another when they are emitted from a gas that is a mixture of the two isotopes.

A key part of the answer will be explored in Part 2 on instrumentation: what design features of spectrometers allows for such discrimination to be done?

Another part of the answer depends on how the gas itself can contribute to broadening. As mentioned near the beginning of this Part 1, two of the processes to consider are:

- Doppler broadening due to thermal motion of the atoms
- Pressure broadening due to frequent collisions between atoms

Future versions of this write-up might provide further guidance on this but in the meantime, you are encouraged to look up such issues in the literature and see what you discover!

# 1.11 Appendix - data for fundamental particles

See for example <a href="https://physics.nist.gov/cgi-bin/cuu/Value?md">https://physics.nist.gov/cgi-bin/cuu/Value?md</a> (<a href="https://physics.nist.gov/cgi-bin/cuu/Value?md">https://physics.nist.gov/cgi-bin/cuu/Value?md</a

#### **Fundamental constants**

$$h = 6.62607015 \times 10^{-34} \text{J s.}$$

$$c = 2.99792458 \times 10^8 \text{ms}^{-1}.$$

$$e = 1.602176634 \times 10^{-19} \text{C.}$$

$$\epsilon_0 = 8.8541878128 \times 10^{-12} \text{N mC}^{-2}.$$

$$\alpha = \frac{1}{2\epsilon_0} \frac{e^2}{hc} = \frac{1}{137.035999084}.$$

#### **Useful combinations**

$$hc = 1239.856346 \approx 1240 \text{ eV nm.}$$
  
 $m_e c^2 = .5109989499 \times 10^6 \text{ eV.}$ 

#### **Masses**

$$M_{D^{+}} = 3.3435837724 \times 10^{-27} \text{Kg}$$
  
 $M_{p} = 1.67262192369 \times 10^{-27} \text{Kg}$   
 $M_{n} = 1.67492749804 \times 10^{-27} \text{Kg}$   
 $m_{e} = 9.1093837015 \times 10^{-31} \text{Kg}$   
 $Mp + Mn - M_{D^{+}} = 0.0039656493 \text{Kg}$ 

#### **Mass ratios**

$$\frac{M_{D^{+}}}{Mp} = 1.9990075014$$

$$\frac{M_{p}}{m_{e}} = 1836.1526734$$

$$\frac{m_{e}}{M_{p}} = 0.0005446170215$$

$$\frac{m_{e}}{M_{D^{+}}} = 0.0002724437107$$

#### **Rydberg constant**

$$R_{\rm m} = 1.0973731568160 \times 10^7 \,\mathrm{m}^{-1}$$
.

 $a_0 = 5.29177210903 \times 10^{-11} \text{ m} = 0.0529177210903 \text{ nm}.$ 

# 1.12 References

#### **1.12.1 Websites**

Hydrogen spectral series <a href="https://en.wikipedia.org/wiki/Hydrogen\_spectral\_series">https://en.wikipedia.org/wiki/Hydrogen\_spectral\_series</a> <a href="https://en.wikipedia.org/wiki/Hydrogen\_spectral\_series">https://en.wiki/Hydrogen\_series</a> <a href="https://en.wiki/Hydrogen\_spectral\_series">https://en.wiki/Hydrogen\_series</a> <a href="https://en.wiki/Hydrogen\_spectral\_series">https://en.wiki/Hydrogen\_series</a> <a href="https://en.wiki/Hydrogen\_spectral\_series">https://en.wiki/Hydrogen\_series</a> <a href="https://en.wiki/Hydrogen\_spectral\_series">https://en.wiki/Hydrogen\_series</a> <a href="https://en.wiki/Hydrogen\_spectral\_series</a> <a href="https://en.wiki/Hydro

# 1.12.2 Journal papers

- S. P. Pollack and E. Y. Wong, "Experiment on hydrogen and deuterium fine structure," Am. J. Phys. **39**, 1386 (1971).
- S. George, "Determination of m, e/m, and Mp/m by the study of the isotope structure in hydrogen," Am. J. Phys. **43**, 885-887 (1975).
- J. Blue, S. B. Bayram and S. D.Marcum, "Creating, implementing, and sustaining an advanced optical spectroscopy laboratory course," Am. J. Phys. **78**, 503-509 (2010).

$$\frac{r_0}{t_0}\frac{d\mathbf{r'}}{dt'}=\frac{1}{m}p_0\mathbf{p'}.$$

$$\frac{p_0}{t_0}\frac{d\mathbf{p'}}{dt'} = -\frac{1}{r_0^2}\frac{e^2}{4\pi\epsilon_0 r'^2}\hat{\mathbf{r}}.$$

So assuming all of the primed quantities are of order unity and neglecting signs,

$$\frac{r_0}{t_0} = \frac{1}{m}p_0.$$

$$\frac{p_0}{t_0} = \frac{e^2}{4\pi\epsilon_0} \frac{1}{r_0^2}.$$