# Isotope Shift of Hydrogen and Deuterium

Practical Course M I. Physikalisches Institut Universiät zu Köln

October 23, 2013

## **Contents**



## <span id="page-2-0"></span>**1 Introduction**

Isotope Shift is called the change in the energy levels of electrons in atoms or molecules that occurs for different isotopes. For lightweight atoms the change in the energy levels of the electrons is mainly caused by the different masses of the nuclei of different isotopes (mass effect). For heavier atoms the charge distribution in the nucleus changes for different numbers of neutrons, and this in turn changes the energy levels of the electrons (volume effect). In addition, different isotopes usually have different nuclear spins. This also contributes to a change in the electron energy levels.

The energy shift between the Hydrogen and the Deuterium isotope can be explained with the mass effect. The change in wavelength of the corresponding spectral lines is  $1-2$  Å, which is large enough to be detected with a medium resolution spectrometer.

## <span id="page-2-1"></span>**2 The Hydrogen Atom**

#### <span id="page-2-2"></span>**2.1 Bohr–Sommerfeld Model**

The basic characteristics of the Hydrogen spectrum can be explained with the Bohr model [\[1\]](#page-19-1). For the energy levels  $E_n$  one finds:

$$
E_n = -R_{\infty}/n^2,\tag{1}
$$

with  $n = 1, 2, 3, \ldots$  and the Rydberg constant  $R_\infty = 13.605$  eV. In Bohr's model of the atom, the isotopic shift caused by a change in the mass of the atomic nucleus can be explained as follows: The Rydberg constant  $R_{\infty}$  is determined for a static atomic nucleus (i.e. with an infinite mass), which is then proportional to the electron mass  $m_e$ . A more realistic approach models the atom as a classical two-body problem, in which both the nucleus and the electron are moving. In the solution of the two-body problem,  $m_e$  is substituted by the reduced mass  $\mu$  given by:

$$
\mu = \frac{m_e \cdot m_k}{m_e + m_k},\tag{2}
$$

with  $m_k$  the mass of the nucleus.

In Bohr's model of the atom, electron states with zero orbital angular momentum do not exist. This problem is solved by a description of the atom using the Schroedinger equation [\[2](#page-19-2)]. In the Schroedinger equation, however, the spin of the electron is still not taken into consideration. This is done by the Dirac equation that describes fine-structure and relativistic effects. The solution of the Dirac equation still needs to be corrected for quantum-electrodynamical effects in order to be able to explain the Lamb-shift.

#### <span id="page-2-3"></span>**2.2 Schroedinger equation for the Hydrogen atom**

The Hamiltonian including only the Coulomb interaction is given by:

$$
\hat{H} = \frac{1}{2m_k} \hat{P}_k^2 + \frac{1}{2m_e} \hat{P}_e^2 - \frac{e^2}{|R_k - R_e|},\tag{3}
$$

where  $\hat{P}$  and  $\hat{R}$  are the operators of the momentum and the position, respectively. The first two terms give the kinetic energy of the nucleus and the electron, and the last term describes their Coulomb interaction.



Figure 1: Energy levels and series of spectra for Hydrogen according to the Bohr model.

The solution of the Schroedinger equation

$$
\hat{H}|\Psi\rangle = E|\Psi\rangle \tag{4}
$$

gives the eigenvectors  $|\Psi\rangle$  und energy eigenvalues *E* of the atom. The equation can be simplified by introducing coordinates relative to the center of gravity of the atom.  $\hat{H}$  is then written as:

$$
\hat{H} = \frac{1}{2(m_e + m_k)} \hat{P}_s^2 + \frac{1}{2\mu} \hat{P}_{ke}^2 - \frac{e^2}{R_{ke}},
$$
\n(5)

with  $\hat{P}_s$  and  $\hat{P}_{ke}$ , respectively, the momentum operator of the nucleus and the electron in the new coordinate system, and *R*ke the absolute value of the position operator. Because of  $\hat{H} = \hat{H}_s + \hat{H}_{ke}$ ,  $|\Psi\rangle$  can be split in two dynamically independent parts:

$$
|\Psi\rangle = |\Psi_s\rangle |\Psi_{ke}\rangle. \tag{6}
$$

To determine the isotopic shift, only  $|\Psi_{ke}\rangle$  is of interest, which describes a particle with mass  $\mu$  in a central potential field of  $e^2/r$ .

Since this a problem of spherical symmetry, the angular momentum is a constant of motion. The state vectors that are a solution of the Schroedinger equation are then characterized by the quantum numbers *E*, *l* and *m<sup>l</sup>* :

$$
|\Psi\rangle_{ke} = |E, l, m_l\rangle. \tag{7}
$$

The eigenvalues of the operators  $\hat{H}$ ,  $\hat{L}^2$  and  $\hat{L}_z$  are  $E$ , *n*,  $l(l+1)$  und  $m_l$  [\[2](#page-19-2)]. The solution of the Schroedinger equation can be obtained in the following steps: (The index *ke* will be omitted from here on)

• Using the position representation, the equation is changed from an operator equation into a differential equation. Because of the sperical symmetry of the potential term, spherical position coordinates are used.

<span id="page-4-0"></span>
$$
\langle r|\hat{H} - E|E, l, m_l \rangle = \left(-\frac{\hbar^2}{2\mu}\Delta - \frac{e^2}{r} - E\right) \langle r|E, l, m_l \rangle \tag{8}
$$

with

$$
\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \theta^2} \right].
$$
 (9)

• The part of the Laplace operator  $\Delta$  that depends on  $\theta$  and  $\phi$  is equal to the operator 1  $\frac{1}{h^2}\hat{L}^2$  in the position representation. The effect of  $\frac{1}{h^2}\hat{L}^2$  on *E*, *l*, *m<sub>l</sub>* is known, and it is used to rewrite eq. [\(8\)](#page-4-0) as:

<span id="page-4-1"></span>
$$
\left(-\frac{\hbar^2}{2\mu}\Delta - \frac{e^2}{r}\right)\langle r|E, l, m_l\rangle =
$$
\n
$$
\left[-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)\frac{\hbar^2l(l+1)}{2\mu r^2} - \frac{e^2}{r} - E\right]\langle r|E, l, m_l\rangle.
$$
\n(10)

From eq. [\(10\)](#page-4-1) it can be seen that the wave function  $\langle r|E, l, m_l \rangle$  can be separated in two parts, one part depending only on the radius *r*, and the other only on the angular coordinates.

$$
\langle r|E, l, m_l \rangle = R(r) \cdot \chi(\theta, \phi) \tag{11}
$$

• The solution of the equation for the radius gives the radial part of the wave function and the possible energy eigenvalues. For states with energy  $(E < 0)$ :

$$
E_n = -\frac{R_H}{n^2}, \quad \text{with} \quad n = 1, 2, 3, \dots \quad (\equiv \text{principal quantum number}) \tag{12}
$$

These energy eigenvalues are degenerate (which means that there is more than one wave function for the same energy eigenvalue). For example, all wave functions for a certain quantum number *n* have the same eigenvalue  $E_n$  for all quantum numbers *l*, with  $l + 1 \le n$ (*l*-degeneracy). In addition, the problem is rotation invariant, which causes a  $m_l$ -degeneracy (degeneracy of 2*l*+1). As a consequence, every energy eigenvalue  $E_n$  has  $\sum_{l=0}^{n-1} 2l + 1 = n^2$ different wave functions.

In spectroscopy it is common practice to label states with the principal quantum number *n* and with an alphabetic character that comprises the angular momentum quantum number *l*. The following symbols are used:

<span id="page-4-2"></span>
$$
l = 0, 1, 2, 3, 4, 5, \dots
$$
  
s, p, d, f, g, h, \dots etc. in alphabetic order (13)

#### <span id="page-5-0"></span>**2.3 Probability density of the electron position**

In the quantum mechanical description of the Hydrogen atom, the electrons do not circle in defined orbits anymore. There is a probability density for the electrons around the nucleus. This density has a characteristic form for every wave function. The probability to find an electron in a certain element of space  $d^3r$  at position *r* is given by [\[2](#page-19-2)]:

$$
|\langle \vec{r}|E_n, l, m_l \rangle|^2 d^3 r \tag{14}
$$

Because according to eq. [\(10\)](#page-4-1) the wave function can be separated into a radial part and an angular part, also the probability density can be separated in these two parts.



<span id="page-5-2"></span>Figure 2: Radial part of the wave function for the three lowest energy levels

From the graph of the radial part of the wave function  $R_{n,l}(r)$  in Fig. [2](#page-5-2) (the function only depends on the quantum numbers *n* und *l*), it is clear that the expression  $R_{n,0}(r)R_n^*$  $n<sub>n,0</sub>(r)$  does not vanish for *r* approaching zero. This suggests that there is a non-zero probability that the position of the *s*-electrons is inside the nucleus. If the probability for the electron to be found in a spherical shell with radius *r* between *r* and  $r + dr$  is calculated from  $R_{n,l}(r)R_n^*$  $\int_{n,l}^{*}(r)r^{2}dr,$ the result is as shown in Fig. [3.](#page-6-1)

#### <span id="page-5-1"></span>**2.4 Angular part of the wave function**

The angular parts of the wavefunctions of Hydrogen are given by the spherical harmonic functions  $Y_{l,m}(\theta, \phi)$ . The probability density  $Y_{l,m}Y_{l,m}^*$  $\int_{l,m}^{*} d\phi$  is with  $Y_{l,m} \propto \exp(im\phi)$  independent of the azimuthal angle  $\phi$ , i.e. it is rotational symmetric around the *z*-axis.

Its dependence on  $\theta$ , which gives the probability to find the electron in a spherical shell with its half opening angle between  $\theta$  and  $\theta + d\theta$ , is given by  $Y_{l,m}Y_{l,m}^*$  $\int_{l,m}^{*} \sin \theta d\theta$ , shown in Fig. [4](#page-6-2) and Fig. [5.](#page-7-0)

A graph that combines the angular and the radial dependence to a 3D plot of the probability density is shown in Fig. [6](#page-8-0) and Fig. [7.](#page-9-0) In these figures, the brightness of the "cloud" gives the probability to find the electron at that position. A brighter cloud means a higher probability.



<span id="page-6-1"></span>Figure 3: Radial position probability density for the electron in the three lowest energy levels



<span id="page-6-2"></span>Figure 4: Angular part of the wave function of the electron in the *p*-state  $(l = 1)$ . (Source: http://www.tf.uni-kiel.de/matwis/amat/mw1\_ge/kap\_2/backbone/r2\_1\_4.html)

#### <span id="page-6-0"></span>**2.5 Corrections**

The degeneracy of the Hydrogen energy eigenstates is removed when, in addition to relativistic effects and corrections originating from quantum electrodynamics, the interactions between electron spin, nuclear spin, and angular momentum are taken into consideration. That means that the following corrections (given in order of size) must be added to the solution of the Schroedinger equation (see Section [2.2\)](#page-2-3):

- 1. Interaction between the magnetic moment caused by the electron spin and the magnetic moment caused by the electron orbit (spin-orbit coupling)
- 2. Relativistic change of the electron mass and corrections due to the uncertainty of the electron orbit, which causes a deviation of the 1/*r* potential.

Effects 1 and 2 are the origin of the so-called "fine-structure".



<span id="page-7-0"></span>Figure 5: Angular part of the wave function of the electron in the  $d$ -state  $(l = 2)$ . (Source: http://www.tf.uni-kiel.de/matwis/amat/mw1\_ge/kap\_2/backbone/r2\_1\_4.html)

- 3. Interaction between the magnetic moment of the nuclear spin and the total magnetic moment of electron spin and electron orbit. This effect causes the "hyperfine-structure".
- 4. Small corrections originating from quantum electrodynamics due to vacuum polarisation and zero point fluctuations of the radiation. These effects cause the "Lamb-shift".

For further study of the effects mentioned in points 3 and 4, one is referred to [\[2](#page-19-2)]. Concerning the fine structure it can be shown that the correction for the relativistic changes of the mass removes the *l*-degeneracy.

The spin-orbit coupling can be understood starting from classical considerations, see also [\[2\]](#page-19-2). After removing the *l*-degeneracy by implementing the relativistic corrections, the energy eigenvalues are given by *En*,*<sup>l</sup>* . These energy values need to be corrected for the energy that is connected with the orientation of the magnetic moment related to the spin of the electron in the magnetic field that is generated at the position of the electron by the orbit of the electron. Classically this energy is given by:

<span id="page-7-1"></span>
$$
\Delta E = \frac{1}{2m^2c^2} \frac{e^2}{r^3} (\vec{L} \cdot \vec{S}),
$$
\n(15)

where *r* is the radius of the electron orbit,  $\vec{L}$  is angular momentum of the electron orbit, and  $\vec{S}$  is the spin vector of the electron. From eq. [\(15\)](#page-7-1) it is clear that the energy correction depends on the relative orientation of  $\vec{L}$  and  $\vec{S}$ .



<span id="page-8-0"></span>Figure 6: 3D graph of the electronic wave function for the  $2p$ -states ( $n = 2$ ,  $l = 1$ , left column), the 3*p*-states ( $n = 3$ ,  $l = 1$ , center column), and the 3*d*-states ( $n = 3$ ,  $l = 2$ , right column). The corresponding magnetic quantum numbers are  $m = 0$  (upper row),  $m = 1$  (center row), and  $m = 2$  (lower row).

(Source: http://abulafia.mt.ic.ac.uk/Bulatov/gallery/qmech/hydr/index.html)

To translate this energy correction to quantum mechanics, the correspondence principle is used in eq. [\(15\)](#page-7-1). This leads to an additional term in the Hamilton operator,  $\hat{H}_{\text{Spin-Bohn}}$ , being:

$$
\hat{H}_{\text{Spin-Bohn}} = \frac{1}{2m^2c^2} \frac{e^2}{r^3} \hat{L} \cdot \hat{S}
$$
\n(16)

 $(\hat{L}$ : operator of the angular momentum,  $\hat{S}$ : spin operator).



<span id="page-9-0"></span>Figure 7: 3D graph of the electronic wave function for the  $4p$ -states ( $n = 4$ ,  $l = 1$ , left column), the 4*d*-states ( $n = 4$ ,  $l = 2$ , center column), and the 4*f*-states ( $n = 4$ ,  $l = 3$ , right column). The corresponding magnetic quantum numbers are  $m = 0$  (upper row),  $m = 1$  (second row),  $m = 2$ (third row), and  $m = 3$  (lower row).

(Source: http://abulafia.mt.ic.ac.uk/Bulatov/gallery/qmech/hydr/index.html)



<span id="page-10-0"></span>Figure 8: Fine-structure of the three lowest energy levels of atomic Hydrogen.

The contribution of this term of the Hamilton operator is generally being calculated with the perturbation method. The result of this calculation is shown in Fig. [8.](#page-10-0)

All states with  $l \neq 0$  are spilt into doublets that correspond to a "parallel" and an "anti-parallel" orientation of orbital angluar momentum and spin. The spectroscopical notation for states that belong to the principal quantum number *n* with  $\vec{L}$  and  $\vec{S}$  coupled to a total angular momentum  $\vec{J}$  is:

$$
n^{2s+1}L_j \quad \text{z.B.} \quad 4^2F_{7/2}.\tag{17}
$$

*s*,*L*, *j* are the quantum numbers of the spin and both angular momentums. For the notation of *L* see eq. [\(13\)](#page-4-2).

If the relativistic correction of the energy and the spin-orbit correction are both applied, it appears that the energy of states with the same *j* is identical (see Fig. [8\)](#page-10-0). This means that now there is a *j*-degeneracy that is removed again by applying the "Lamb-shift" correction.

## <span id="page-11-0"></span>**3 Selection Rules, Line Width**

The position of the energy levels of the electrons is determined experimentally by analysis of the spectrum of the electromagnetic radiation emitted due to electronic transistions between the energy levels. The allowed transitions are given by the selection rules, which are determined from the conservation laws to which the transitions need to comply.  $(i: initial state of the atom, f: final state of the atom):$ 

- 1. Energy conservation law  $E_i = E_f + hv$  (*v*: frequency of the radiation)
- 2. Conservation of angular momentum  $\vec{J}_i = \vec{J}_f + \vec{J}_{\text{Radiation}}$ or  $|\vec{J}_i - \vec{J}_f| \leq \vec{J}_{\text{Radiation}} \leq |\vec{J}_i + \vec{J}_f|$ |
- 3. Parity conservation

 $(Parity)_i = (Parity)_f \cdot (Parity)_{radiation}$ 

The parity gives the symmetry of the wave function when it is mirrored with respect to the origin of the coordinate system:

pos. (+) Parity  $\leftrightarrow$  no sign change

neg. (−) Parity ↔ sign change

Wave functions that are physically meaningful have a parity (with exception of wave functions, where the weak interaction plays a role (e.g.  $\beta$ -decay))

The momentum as a property of the electromagnetic radiation has a relation to its multipolarity  $2^l$ . *l* indicates the angular momentum (e.g.  $2^l$  dipole radiation – angular momentum 1,  $2^2$  quadrupol radiation – angular momentum 2). The parity of the radiation is determined by its angular momentum and its character (either electronic (E) radiation or magnetic (M) radiation):

For E–radiation: Parity  $(-1)^l$ 

For M–radiation: Parity (−1)*l*+<sup>1</sup>

If there is more than one possible radiation type in the transition between two energy levels, the different radiation types are observed according to their transition probability. About the transition probability one can say (qualitatively): "The transition probability decreases with increasing multipolarity. At the same level of multipolarity, the transition probability is smaller for M–radiation than for E–radiation."

It follows that E–dipole radiation has the highest probability. For this radiation the selection rules are:

$$
\Delta J = 0, \pm 1, \quad \text{but not} \quad 0 \to 0 \tag{18}
$$

$$
\Delta l = \pm 1,\tag{19}
$$

$$
\Delta m_j = 0, \pm 1. \tag{20}
$$

Transitions that are only possible via other radiation types than E–dipole radiation are labelled as forbidden, because they have a much smaller transition probability than the E– dipole radiation.

#### <span id="page-12-0"></span>**3.1 Line width**

In an experimental setup one will not be able to observe "sharp"(delta function like) wavelength or frequency signals, even using an instrument (spectrometer) with an extremely high resolution. One always observes a distribution of wavelengths or frequencies. The reasons for this observation are the different physical mechanisms that lead to broadening of the lines, i.e. natural line width, Doppler broadening, pressure broadening.

If one could observe the spectrum of spontaneous emission of atoms that do not move and that have no interaction with other atoms, the line width of the observed lines would be the natural line width. The natural line width is related to the life time  $(= 1/transition probability)$ of the atomic state via a Fourier transformation. Approximately:

$$
\Gamma \cdot \tau \sim \hbar \qquad (\Gamma : \text{nat. line width, } \tau : \text{ life time}) \tag{21}
$$

The natural line width for transitions with wavelengths in the visible spectrum that have a life time of around  $10^{-8}$  s is approximately  $10^{-4}$  Å. Consequently, at room temperature, it is much smaller than the Doppler broadening. A convolution of the Doppler shift with the thermal velocity distribution gives for the line width:

$$
\delta v_D = \frac{2v_0}{c} \sqrt{\frac{2RT\ln 2}{M}} = 7.16 \times 10^{-6} v_0 \sqrt{\frac{T}{M}}
$$
 (22)

( $v_0$ : atomic frequency, *M*: atomic mass, *T*: temperature [K], *R*: gas constant) At room temperature the line width of a Doppler-broadened line of Hydrogen in the visible spectrum is approximately 0.6 Å.

### <span id="page-12-1"></span>**4 Isotope Shift**

There are two main causes for the isotope shift, the volume effect and the mass effect. The volume effect dominates the mass effect for heavy atoms. The larger nucleus expands, which changes the 1/*r* potential field. For isotopes this expansion depends, with a constant number of protons in the nucleus, on the different number of neutrons in the nucleus, which changes the charge density in the nucleus and the potential field accordingly. This effect will be the strongest for the *s*-electrons. The mass effect will dominate for the lighter atoms and their isotopes. For low-mass nuclei the effect of a different number of neutrons has a large influence on the reduced mass in the Hamilton operator. The mass effect explains the isotope shift of Hydrogen/Deuterium quite well. Because this shift is quite large, approximately 1  $\AA$ , it can be observed also in the case of Doppler-broadened lines.

An estimate of the isotope shift can be obtained from:

 $(R_H$  und  $R_D$  are the Rydberg constants for Hydrogen and Deuterium, respectively)

$$
\frac{R_D}{R_H} = \frac{1 + \frac{m_e}{m_H}}{1 + \frac{m_e}{m_D}} \approx \left(1 + \frac{m_e}{m_H}\right) \left(1 - \frac{m_e}{m_D}\right),\tag{23}
$$

or with  $m_D \approx 2m_H$  and  $\frac{m_e}{m_H} \approx \frac{1}{1836}$ :

$$
\frac{R_D}{R_H} \approx 1 + \frac{m_e}{2m_H} = 1 + \frac{1}{2 \cdot 1836}
$$
 (24)

and

$$
\nu_D = R_D \left( \frac{1}{n^2} - \frac{1}{n^2} \right) = R_H \left( 1 + \frac{m_e}{2m_H} \right) \left( \frac{1}{n^2} - \frac{1}{n^2} \right) \tag{25}
$$

$$
= \nu_H \left( 1 + \frac{1}{2.1836} \right) \tag{26}
$$

or

$$
\lambda_D = \lambda_H \left( 1 - \frac{1}{2 \cdot 1836} \right) \tag{27}
$$

and

$$
\Delta \lambda = \lambda_H - \lambda_D = \lambda_H \frac{1}{2 \cdot 1836}.
$$
\n(28)

It is clear that the Deuterium lines are shifted to shorter wavelengths. The magnitude of the shift is proportional to the wavelength.

## <span id="page-13-1"></span><span id="page-13-0"></span>**5 Instrumentation**

#### **5.1 The Grating Spectrometer**

To observe the isotopic shift between Hydrogen and Deuterium, a resolution of  $\lambda/\Delta\lambda \ge 10^4$ is necessary. This resolution can be realized with a good grating spectrometer, that is usually equipped with a reflection grating. For a flat grating with grating constant (grating parameter) *a* it holds for the intensity maximum of order *n* that:

$$
n\lambda = a(\sin \alpha - \sin \beta). \tag{29}
$$

From this equation one obtains, for a constant angle of incidence  $\alpha$ , for the angular dispersion:

$$
\frac{d\beta}{d\lambda} = -\frac{n}{a\cos\beta} = -\frac{\sin\alpha - \sin\beta}{\lambda\cos\beta}.
$$
\n(30)

The optical path through the spectrometer is shown in Fig. [9.](#page-14-0) Fig. [10](#page-14-1) shows a photograph of the grating in the spectrometer.

The divergent optical beam that originates from the entrance slit is collimated by the first parabolic mirror in such a way that a plane wave is generated at the grating. After reflection on the grating, the light is focused on the output slit by a second parabolic mirror. Behind the output slit a photomultiplier is placed as detector.

The resolution of a grating is theoretically given by:

$$
\frac{\lambda}{\Delta \lambda} = n \cdot N,\tag{31}
$$

where *N* is the number of lines on the grating that contribute to the interference pattern.

In practice the achieved resolution of a grating depends mainly on the way the light falls onto the grating. Grating lines that are not getting enough (or any) light do not (fully) contribute to the final interference pattern. They reduce the actual value of *N*, and consequently the resolution. The width of the light beam that falls onto the grating is determined by the interference at the entrance slit. This is shown schematically in Fig. [11.](#page-15-2) To be on the safe side, for a maximum resolution a very small entrance slit would be the right choice. The disadvantage of that is that a small entrance slit greatly reduces the light intensity that enters the spectrometer. This means that in practice one has to find a compromise between resolution and intensity.



<span id="page-14-0"></span>Figure 9: Schematical optical path inside the grating spectrometer. The grating is rotated around its vertical axis to select the wavelength of constructive interference, that is directed towards the output slit.

<span id="page-14-1"></span>

Figure 10: Photograph of the inside of the spectrometer. In the center of the picture, one sees the grating with the drive-mechanism in front. The two boxes in the far corners are the entrance slit and the output slit.



<span id="page-15-2"></span>Figure 11: Relation between entrance slit width (X-axis) and measured line width (Y-axis). The inserts show the corresponding illumination of the grating

#### <span id="page-15-0"></span>**5.2 Calibration Source**

Before the actual measurement of the Hygrogen/Deuterium isotopic shift, the wavelength scale of the spectrometer is calibrated by using a Hg/Cd calibration light source. This lamp emits 12 well defined spectral lines with known frequencies (please see Table [1\)](#page-15-3) that cover the frequency range that later is needed for the detection of the  $\alpha - \delta$  lines of the Balmer series of Hydrogen/Deuterium.

Table 1. Table of calibration wavelengths											
	Nr. $1 \t 2 \t 3 \t 4 \t 5 \t 1$										
	$\lambda/\text{\AA}$ 4046.6 4077.8 4358.4 4414.6 4678.2 4799.9										
	Nr. 7 8 9 10 11 2										
	$\lambda/\text{\AA}$ 4916.0 5085.5 5460.7 5769.6 5790.7 6438.5										

<span id="page-15-3"></span>Table 1: Table of calibration wavelengths

#### <span id="page-15-1"></span>**5.3 H**/**D-source**

To generate the Hydrogen/Deuterium spectral lines a discharge tube is used (see Fig. [12\)](#page-16-2), that should only be used in the *vertical* position. It contains a mixture of  $H_2O$  and  $D_2O$ . After a short warm up time (approx. 5 min) the lamp should burn steadily.



<span id="page-16-2"></span>Figure 12: Hydrogen/Deuterium discharge source with the condensor lense in front.

#### <span id="page-16-0"></span>**5.4 Light Detector**

The detector at the output slit is a photomultiplier. It generates a current as measure of the light intensity, which is measured by a picoampere meter (Fig. [13\)](#page-17-0) that is interfaced with a computer by an AD-converter for data acquisition. To minimize the bit noise in the digitalized signal, the picoampere meter should be adjusted for each measurement in such a way that the largest possible sensitivity is used. (This means that on the analog front display of the picoampere meter the needle should, of course, not go off scale, but at the same time the sensitivity should be adjusted in such a way that the largest possible portion of the scale is used.) In addition care should be taken to adjust the offset to insure that the needle remains above zero when there is no spectral line signal, because the AD-converter is not able to convert negative voltages.

## <span id="page-16-1"></span>**5.5 Software**

The data acquisition is done by the program "PH1-Spectrometer", see Fig. [14.](#page-17-1) The data acquisition is automatically synchronized with the rotation of the grating during the measurement. The control of the experiment, however, is not done by the computer but it is in your hands. The procedure is as follows: Before the measurement, the grid is positioned in such a way that the wavelength reading on the spectrometer is slightly  $(3-4 \text{ Å})$  below the expected peak value of the line. This start value of the wavelength needs to be typed in into the program by the experimentalist. In addition, a (meaningful) filename has to be chosen and the computer has to be switched to the ready-to-measure state (scan). The actual measurement is started, by you, from the grid motor control by activating the scan switch. The



Figure 13: Photograph of the picoampere meter to measure the detector current

<span id="page-17-0"></span>measurement is ended by the same switch, after checking on the display that the spectral line has been properly measured. The wavelength values are generated automatically from the start value that has been typed in and the number of steps. The data are saved as an ASCII-table.

PH1.Monochromator22.vi 中国			$\Box$ D x	
$0.25 \frac{0.5}{1} \frac{0.75}{1} \frac{1}{1} \frac{1.2}{1} \frac{1.5}{1.5}$ 1,8 $0\,$ SensorSpannung [Volt] 0,652 $2,5 -$	Daten speichern sayt $^{4}$ 4659,6 neue Datei	Kommentar (wird bei jedem Messwert gespeichert) StartWert IstWert Anzahl Messwerte 4666,5 69 in diese Datei wird gespeichert: %D:\Praktikum\AndacJavadi\EICHPEAKS.dat	No Error $\blacktriangle$	
$2,25-$				
$2 -$				
$1,75-$				
$\frac{1}{2}$ 1,5 - $\frac{1}{2}$ 1,25 -				
<b>Sensor</b>				
$1 -$ $0,75 -$				
$0,5 -$				
$0,25 -$				
$\frac{0}{4659,5}$				

<span id="page-17-1"></span>Figure 14: Data acquisition program at the end of the measurement

#### <span id="page-18-0"></span>**5.6 Measurement Equipment**

- Grating: 1200 Lines/mm,  $\lambda_{\text{Blaze}}$ : 5000 Å
- Parabolic mirror: 50mm diameter, 350 mm focal distance
- Slit height: 3 mm
- Slit width: continuously adjustable, 1 mm equals  $\Delta \lambda \approx 20 \text{ Å}$  at 6328 Å
- Rotation of the grating: Step motor, with measurement velocity 0.05  $\rm \AA/s 100$   $\rm \AA/s$ .  $(0.05 \text{ Å/s})$  is recommended for the H/D measurement, 0.1 Å/s for the preceding measurements).
- Photomultiplier: Bias voltage 800 V; Long wavelength sensityity cut off: 7 000  $\AA$
- Picoampere meter: can be used to compensate for the photomultiplier dark current. (Please start measurements at a low sensitivity scale and adjust accordingly afterwards.)

## <span id="page-18-1"></span>**6 TO DO**

- 1. Adjustment of source and condensor outside the spectrometer box
- 2. Determination of the optimum entrance slit width. **Data analysis immediately, during the lab course.**

With the optimum width for the entrance slit:

- 3. Calibration of the wavelength scale
- 4. Measurement of the wavelengths of the  $\alpha$ -,  $\beta$ -,  $\gamma$ -, and  $\delta$ -lines of the Balmer series of Hydrogen and Deuterium
- 5. Data analysis afterwards:
	- Determine the Rydberg constants for H and D from the measured wavelengths; include an analysis of the accuracy of the result.
	- Calculate *me*/*m<sup>H</sup>* from the Rydberg constants, again with accuracy analysis
	- Determine the mass of the Deuterium atom; with accuracy analysis
	- Calculate *e*/*m<sup>e</sup>* using in addition the Faraday constant
	- Compare all experimentally determined values with values given in the literature and discuss the results.

## <span id="page-19-0"></span>**7 Questions**

- 1. Give the Bohr postulates.
- 2. What is the size of the Bohr radius (radius of the first orbit) of the Hydrogen atom?
- 3. What is the size of the radius of the first orbit of  $\mu$ -onic Hydrogen?
- 4. Give the formula that relates energy and wavelength of photons.
- 5. What is the energy range of the photons of visible light?
- 6. Derive the equation for the reduced mass.
- 7. How large is the isotopic shift of the  $n = 3 \rightarrow n = 2$  line of Hydrogen towards Deuterium, calculated with Bohr's model?
- 8. How do interference filters work?
- 9. What is a Fabry Perot Interferometer (FPI)? Is it possible to use a stand alone FPI to do spectroscopy?
- 10. How large can the resolution of a prism spectrometer be (Formula and value for a practical example)?
- 11. How large can the resolution of a grating spectrometer be (Formula and value for a practical example)?
- 12. How large should one choose the entrance slit to just illuminate the whole grating with the main lobe of the slit's diffraction pattern?
- 13. What is a phase grating? Why is that the preferred type of grating for this experiment?
- 14. Why is an image of the radiation source (lamp) projected on the entrance slit with the use of a condensor? What type of optical element is the condensor? What do you think of the possibility to do a successful experiment without the condensor?

## **References**

- <span id="page-19-1"></span>[1] B. Cagnac, J.C. Pebay-Peyroula. *Modern atomic Physics, Part1 Fundamental Principles*. Macmillan, 1975
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