atomic_spectra

April 24, 2016

1 Calculation some features of atomic spectra

This are some example calculations that illustrate some properties of atomic spectra and their relation to the inner construction of atoms

```
In [100]: from scipy.constants import *
```

1.1 Atom spectra and energies in H-Atoms

Fig. : Visible spectrum of H-Atom

1.1.1 Electron Transitions

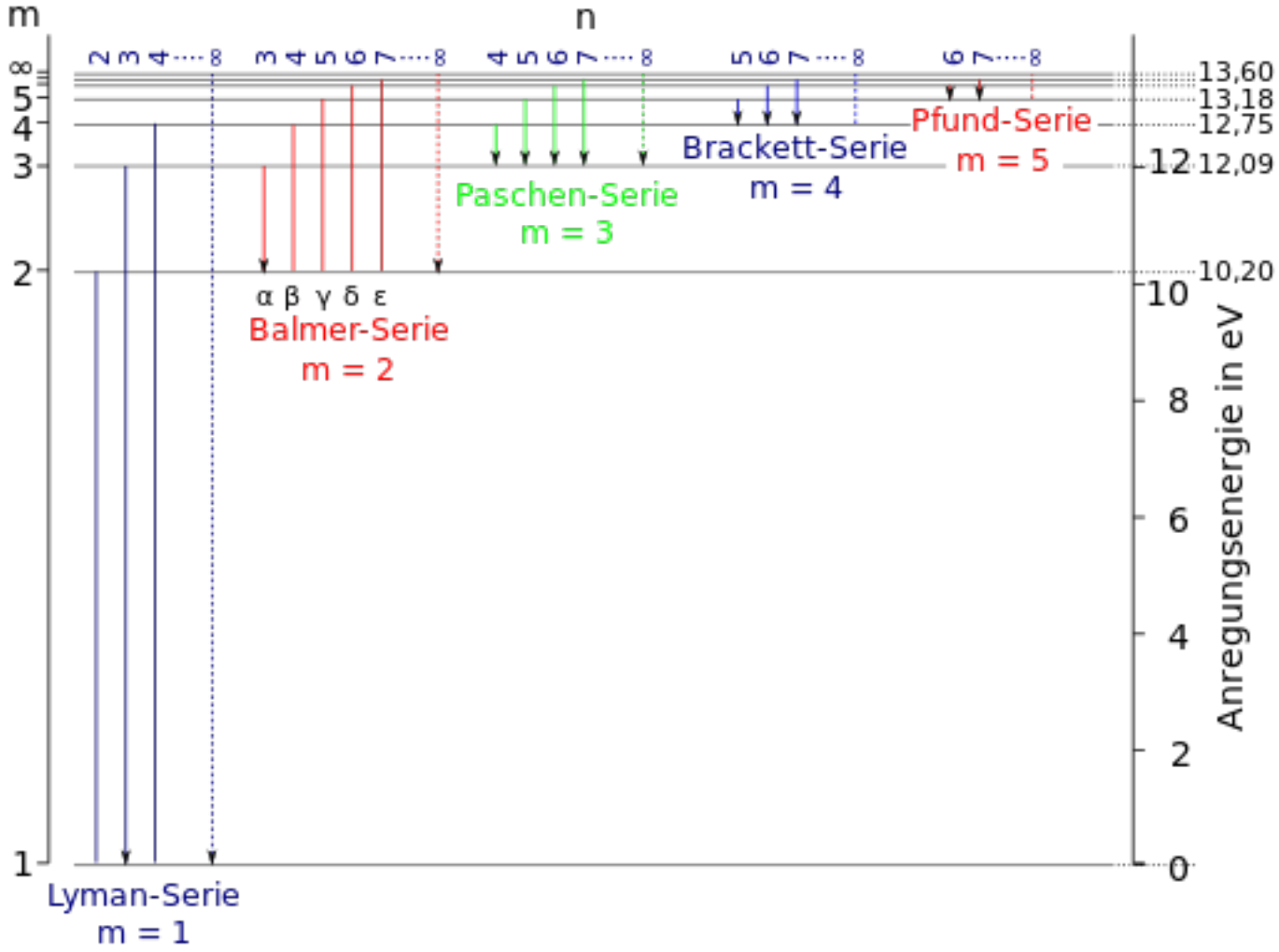

Fig. : Schematic electron transitions in H-atom

→ **energies of atomic orbitals are (destinct and not continous !!) = "qunantized"**

```
In [138]: print( "speed of light in %.1f m/s " % c )
```

```
speed of light in 299792458.0 m/s
```

Relation between Energy and frequency ν of light is given by

$$E = h \cdot \nu$$

where

$$\nu = \frac{1}{\lambda} \cdot c$$

c = speed of light

Example:

```
In [102]: lamda_balmer_alpha = 656.2793e-9 # in m
```

```
In [103]: nu1 = 1 / lamda_balmer_alpha * c
```

```
In [104]: print  "freq. of balmer alpha line: %s Hz" % nu1
```

```
freq. of balmer alpha line: 4.56806207357e+14 Hz
```

or with scipy function lambda2nu()

```
In [105]: lambda2nu(lamda_balmer_alpha)
```

```
Out[105]: 456806207357141.94
```

1.2 Ionisation energy of H-electron

```
In [106]: lambda_lyman_inf = 91.175e-9 # m
```

corresponding energy

```
In [107]: dE_lyman_inf = h * lambda2nu(lambda_lyman_inf)
```

```
In [114]: print "Energy difference %.2f eV (s. Fig. ) " % float(dE_lyman_inf/eV)
```

```
Energy difference 13.60 eV (s. Fig. )
```

1.3 Spectrum of Na atom

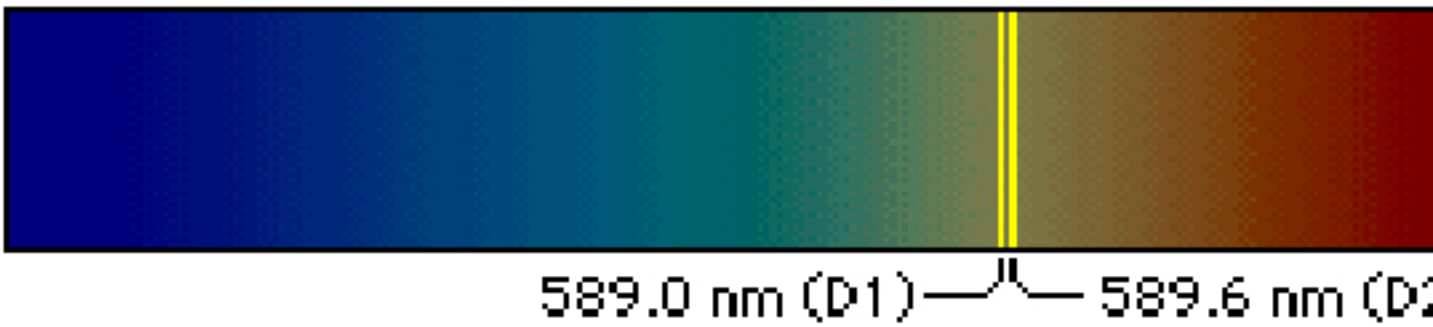

Figure 1: Na-spectrum

Energy difference scheme

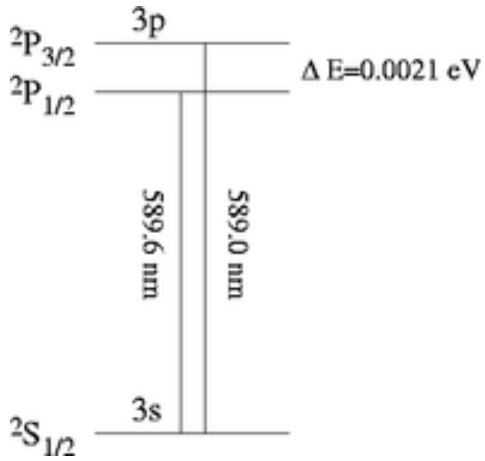

Figure 2: Electron-transitions in Na

```
In [140]: lambdaD1 = 588.9950e-9 # in m
```

```
In [141]: lambdaD2 = 589.5924e-9 # in nm
```

Energy corresponding one line

```
In [142]: dE_D1 = h * lambda2nu(lambdaD1)
```

```
In [143]: print( "Energy difference between 3s and 3p orbital %.3f eV" % (dE_D1/eV) )
```

```
Energy difference between 3s and 3p orbital 2.105 eV
```

```
In [144]: dE_D2 = h * lambda2nu(lambdaD2)
```

```
In [147]: delta_D = dE_D1 - dE_D2
```

```
In [148]: print( "Energy difference between 3p and 3p orbital: %.4f eV" % (delta_D/eV) )
```

```
Energy difference between 3p and 3p orbital: 0.0021 eV
```

Interpretation of this is the spin-pairing energy of the 3p orbital
compare energy differences between different orbitals !