Bohr model of hydrogen

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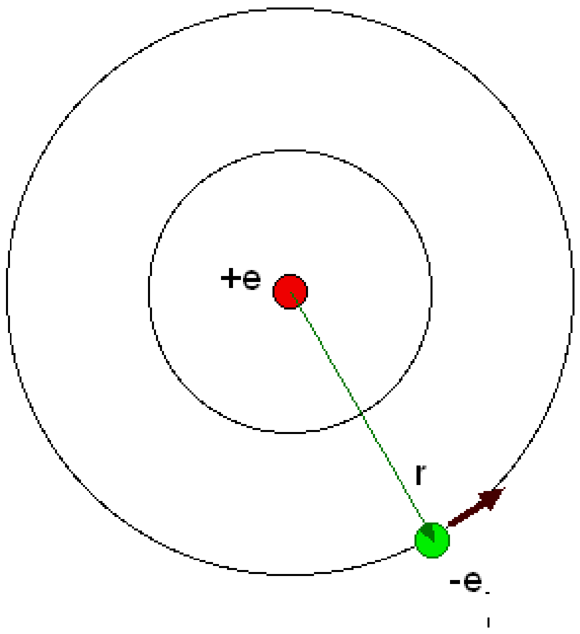
1. Bohr model

We now consider the Bohr model shown in this figure. The system consists of a proton and an electron. These two particles are coupled with an attractive Coulomb interaction.



The total energy is a sum of kinetic energy and potential energy.

$$E = \frac{1}{2}mv^2 - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$m\frac{v^2}{r} = \frac{e^2}{4\pi\varepsilon_0 r^2},$$

or

$$mv^2 r = \frac{e^2}{4\pi\varepsilon_0} \qquad (1)$$

or

$$E = \frac{1}{2}\frac{e^2}{4\pi\varepsilon_0 r} - \frac{e^2}{4\pi\varepsilon_0 r} = -\frac{e^2}{8\pi\varepsilon_0 r}$$

The kinetic energy K is

$$K = \frac{1}{2}mv^2$$

The period T is given by

$$T = \frac{2\pi r}{v} = \frac{2\pi}{\omega}.$$

where ω is the angular frequency.

((**Note**))
The postulate D:

$$K = \frac{nh}{2} f_{orb} = \frac{1}{2}mv^2$$

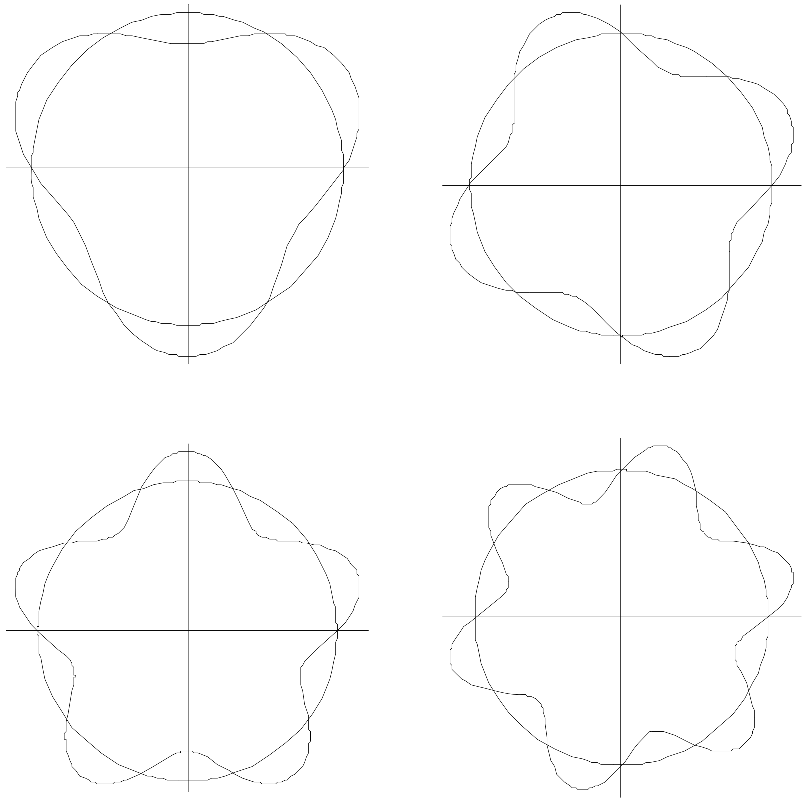
Since

$$f_{orb} = \frac{1}{T} = \frac{v}{2\pi r}$$

we get

$$\frac{nh}{2}\frac{v}{2\pi r} = \frac{1}{2}mv^2, \qquad \text{or} \qquad \frac{n\hbar}{2\pi} = mvr = L$$

This means that the angular momentum is quantized. This relation can be also derived as follows.



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

where n is integer.

de Broglie relation

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

$$p(2\pi r) = \frac{h}{\lambda} 2\pi r = nh$$

The angular momentum L_z:

$$L_z = pr = \frac{nh}{2\pi} = n\hbar \quad \text{or} \quad mvr = n\hbar \qquad (2)$$

The angular momentum is quantized.

From Eqs.(1) and (2),

$$\frac{mv^2 r}{mvr} = \frac{e^2}{n\hbar(4\pi\varepsilon_0)},$$

or

$$v = \frac{1}{n}\frac{e^2}{4\pi\varepsilon_0\hbar} = \frac{1}{n}2.18769\times10^6 \text{ m/s}$$

$$m\left(\frac{e^2}{n4\pi\varepsilon_0\hbar}\right)^2 r = \frac{e^2}{4\pi\varepsilon_0},$$

or

$$r = 4\pi\varepsilon_0 \frac{n^2\hbar^2}{me^2} = n^2 a_0$$

where

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 5.29177 \text{ x } 10^{-11} \text{ m} = 0.529177 \text{ Å}$$

Then the total energy is obtained by

$$E_n = -\frac{e^2}{8\pi\varepsilon_0 n^2 a_0} = -\frac{E_0}{n^2}$$

where

$$E_0 = \frac{e^2}{8\pi\varepsilon_0 a_0} = \frac{e^2}{8\pi\varepsilon_0 \dfrac{4\pi\varepsilon_0\hbar^2}{me^2}} = \frac{me^4}{2(4\pi\varepsilon_0)^2\hbar^2}$$

E_0 =13.6057 eV

The energy is quantized. The ground state is a state with n = 1. The Rydberg constant is defined as

$$R_\infty = \frac{E_0}{hc} = \frac{E_0}{2\pi\hbar c} = \frac{me^4}{4\pi c\hbar^3(4\pi\varepsilon_0)^2} = 1.0973731568539(55) \text{ x } 10^7\text{/m}$$

((Mathematrica))

```
Clear["Global`*"];

rule1 = {me → 9.1093821545 × 10^-31, nm → 10^-9,
    eV → 1.602176487 × 10^-19, u → 1.660538782 × 10^-27,
    qe → 1.602176487 × 10^-19, c → 2.99792458 × 10^8,
    μ0 → 12.566370614 × 10^-7, ϵ0 → 8.854187817 × 10^-12,
    h → 6.62606896 × 10^-34, ℏ → 1.05457162853 × 10^-34,
    mp → 1.672621637 × 10^-27};
```

$$v1 = \frac{qe^2}{4\,\pi\,\epsilon 0\,\hbar\,n} \;\text{//. rule1}$$

$$\frac{2.18769\times 10^{6}}{n}$$

$$a0 = \frac{4\,\pi\,\epsilon 0\,\hbar^2}{me\,qe^2} \;\text{//. rule1}$$

$$5.29177\times 10^{-11}$$

$$r1 = n^2\,a0 \;\text{//. rule1}$$

$$5.29177\times 10^{-11}\,n^2$$

$$T1 = \frac{2\,\pi\,r}{v1} \;\text{//. rule1}$$

$$2.87206\times 10^{-6}\,n\,r$$

$$E1 = -\frac{qe^2}{8\,\pi\,\epsilon 0\,a0\,n^2\,eV} \;\text{//. rule1}$$

$$-\frac{13.6057}{n^2}$$

$$R = \frac{qe^2}{8\,\pi\,\epsilon 0\,a0\,(h\,c)} \;\text{//. rule1}$$

$$1.09737\times 10^{7}$$

2. Hydrogen spectrum

The Bohr model foe an electron transition in hydrogen between quantized energy levele with different quantum number n yields a photon by emission with quantum energy.

$$\hbar\omega = 2\pi\hbar\frac{c}{\lambda} = \frac{hc}{\lambda} = E_m - E_n = E_0(\frac{1}{n^2} - \frac{1}{m^2})$$

or

$$\frac{1}{\lambda} = \frac{E_0}{hc}(\frac{1}{n^2} - \frac{1}{m^2}) = R(\frac{1}{n^2} - \frac{1}{m^2})$$

R is the Rydberg constant.

Lyman series

$$\lambda = \frac{1}{R(\frac{1}{1^2} - \frac{1}{n^2})}$$

Balmer series

$$\lambda = \frac{1}{R(\frac{1}{2^2} - \frac{1}{n^2})}$$

Paschen series

$$\lambda = \frac{1}{R(\frac{1}{3^2} - \frac{1}{n^2})}$$

Brackett series

$$\lambda = \frac{1}{R(\frac{1}{4^2} - \frac{1}{n^2})}$$

Pfund series

$$\lambda = \frac{1}{R(\frac{1}{5^2} - \frac{1}{n^2})}$$

((**Mathematica**))

```
Clear["Global`*"];
rule1 = {R → 10973731.6};
```

$$\lambda Ly[n\_] := \frac{1}{R\left(1-\frac{1}{n^2}\right)} 10^9 \text{ /. rule1;}$$

$$\lambda Ba[n\_] := \frac{1}{R\left(\frac{1}{2^2}-\frac{1}{n^2}\right)} 10^9 \text{ /. rule1;}$$

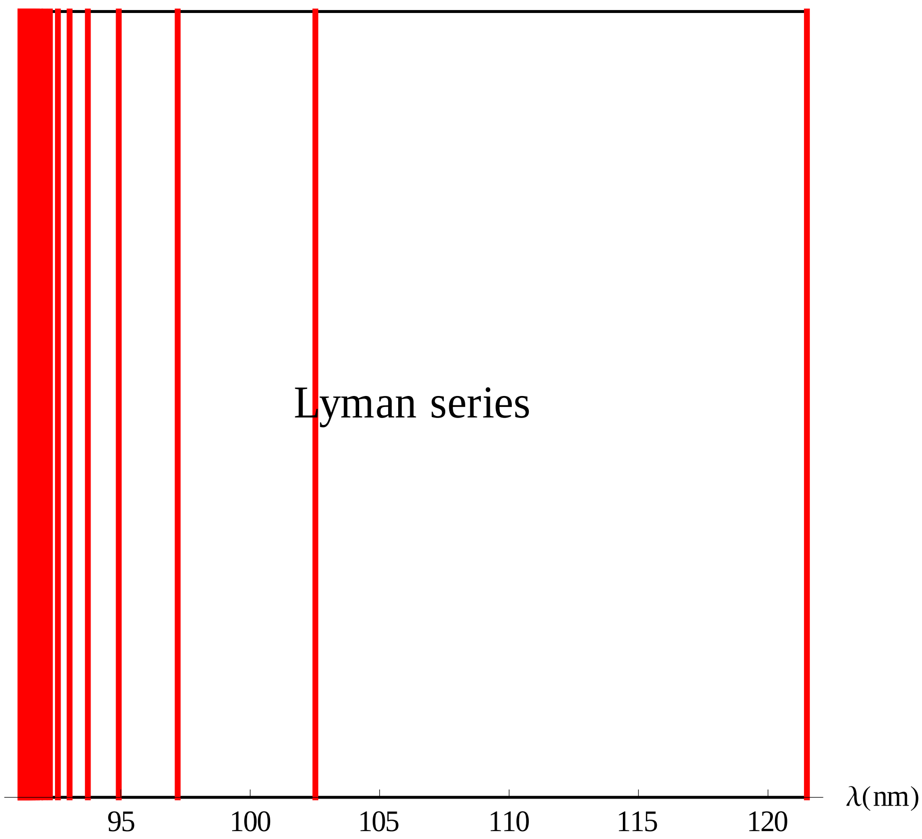
$$\lambda Pa[n\_] := \frac{1}{R\left(\frac{1}{3^2}-\frac{1}{n^2}\right)} 10^9 \text{ /. rule1;}$$

$$\lambda Br[n\_] := \frac{1}{R\left(\frac{1}{4^2}-\frac{1}{n^2}\right)} 10^9 \text{ /. rule1;}$$

$$\lambda Pf[n\_] := \frac{1}{R\left(\frac{1}{5^2}-\frac{1}{n^2}\right)} 10^9 \text{ /. rule1;}$$

Lyman series

```
Nmax = 100; Nmin = 2; K = λLy[Nmin] - λLy[Nmax];
H1 = (λLy[Nmin] + λLy[Nmax]) / 2;
Graphics[
 {Line[{{λLy[Nmax], 0}, {λLy[Nmin], 0}}],
  Line[{{λLy[Nmax], K}, {λLy[Nmin], K}}],
  Hue[0], Thick,
  Table[Line[{{λLy[n], 0}, {λLy[n], K}}],
   {n, 2, 100}],
  Text[Style["Lyman series", Black, 15],
   {H1, K / 2}]}, Axes → {True, False},
 AxesLabel → {"λ(nm)"},
 Ticks → {Range[95, 120, 5]}]
```



```
Prepend[Table[{n, λLy[n] }, {n, 2, 10}],
  {"n", "λLy[nm]"}] // TableForm
```

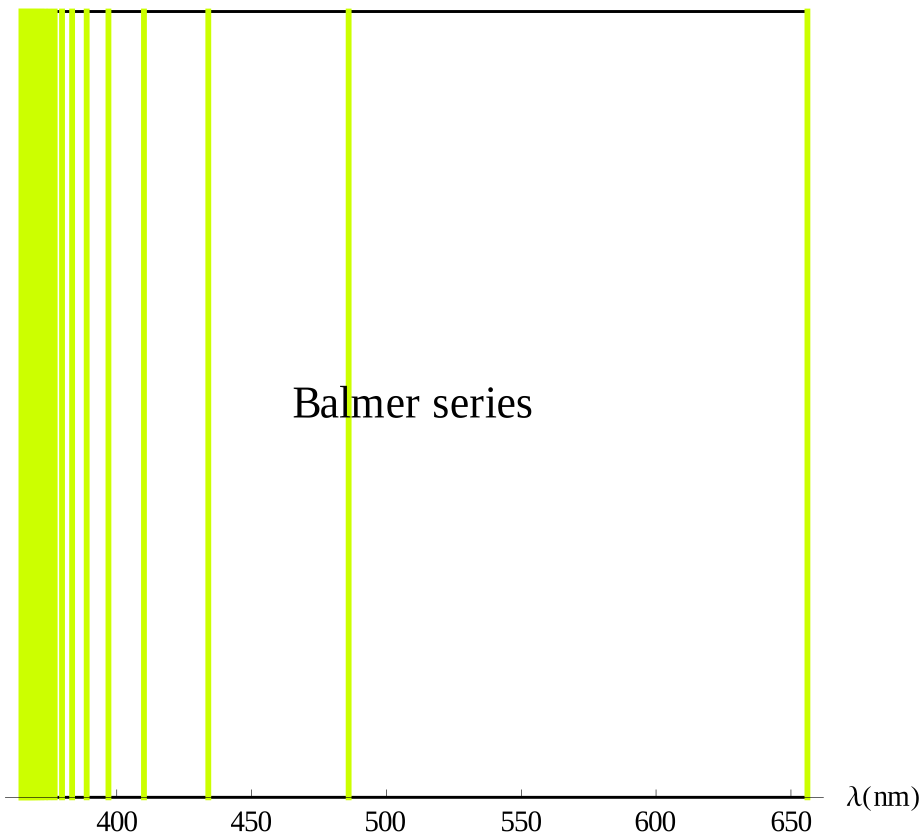
n	λLy[nm]
2	121.502
3	102.518
4	97.2018
5	94.9237
6	93.7303
7	93.0252
8	92.5732
9	92.2658
10	92.0472

```
Limit[λLy[n], n → ∞]
```

91.1267

Balmer series

```
Nmax = 100; Nmin = 3; K = λBa[Nmin] - λBa[Nmax];
H1 = (λBa[Nmin] + λBa[Nmax]) / 2;
Graphics[
 {Line[{{λBa[Nmax], 0}, {λBa[Nmin], 0}}],
  Line[{{λBa[Nmax], K}, {λBa[Nmin], K}}],
  Hue[0.2], , Thick,
  Table[Line[{{λBa[n], 0}, {λBa[n], K}}],
   {n, Nmin, 100}],
  Text[Style["Balmer series", Black, 15],
   {H1, K / 2}]}, Axes → {True, False},
 Ticks → {Range[350, 700, 50]},
 AxesLabel → {"λ(nm)"}]
```



```
Prepend[Table[{n, λBa[n] }, {n, 3, 10}],
  {"n", "λBa[nm]"}] // TableForm
```

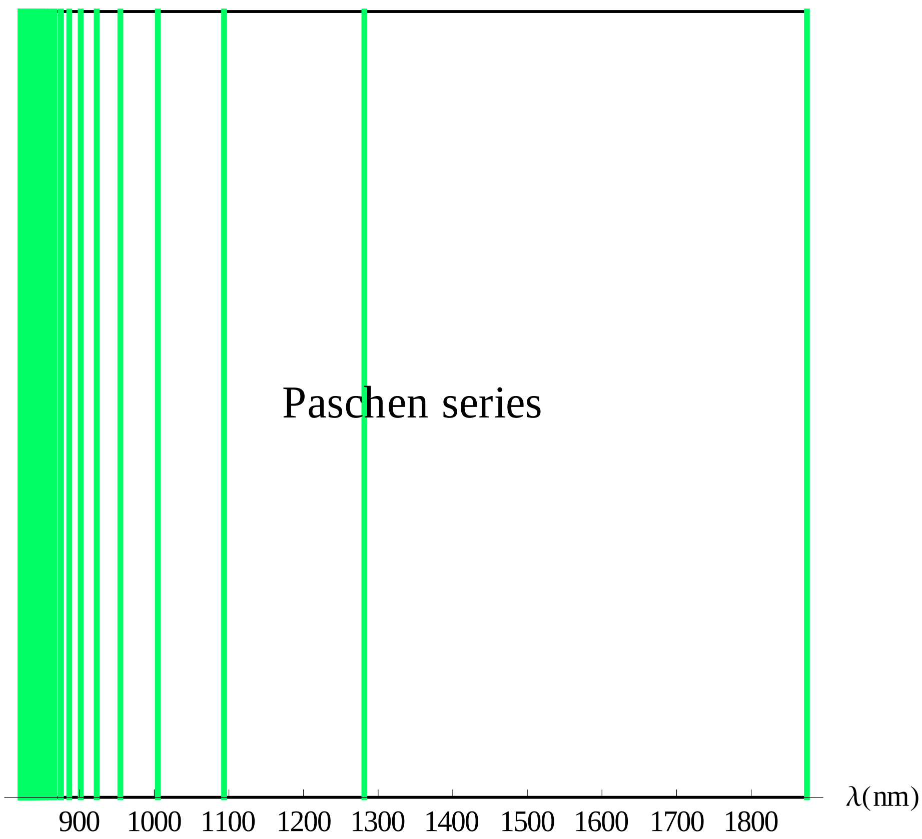
n	λBa[nm]
3	656.112
4	486.009
5	433.937
6	410.07
7	396.907
8	388.807
9	383.442
10	379.695

```
Limit[λBa[n], n → ∞]
```

364.507

Paschen series

```
Nmax = 100; Nmin = 4; K = λPa[Nmin] - λPa[Nmax];
H1 = (λPa[Nmin] + λPa[Nmax]) / 2;
Graphics[
 {Line[{{λPa[Nmax], 0}, {λPa[Nmin], 0}}],
  Line[{{λPa[Nmax], K}, {λPa[Nmin], K}}],
  Hue[0.4], Thick,
  Table[Line[{{λPa[n], 0}, {λPa[n], K}}],
   {n, Nmin, 100}],
  Text[Style["Paschen series", Black, 15],
   {H1, K / 2}]}, Axes → {True, False},
 Ticks → {Range[900, 2000, 100]},
 AxesLabel → {"λ(nm)"}]
```



```
Prepend[Table[{n, λPa[n] }, {n, 4, 10}],
  {"n", "λPa[nm]"}] // TableForm
```

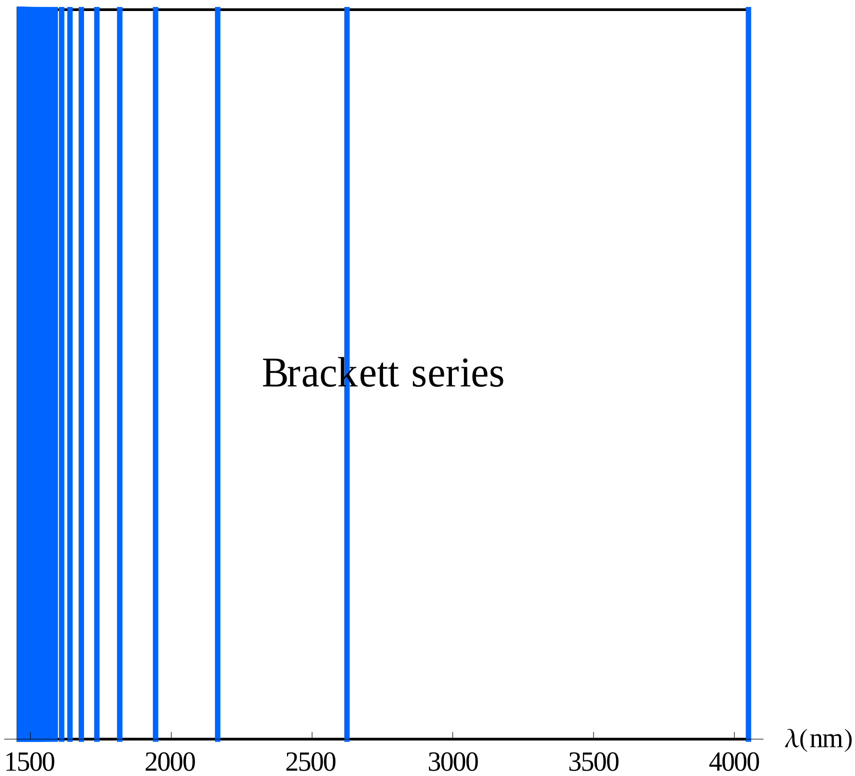
n	λPa[nm]
4	1874.61
5	1281.47
6	1093.52
7	1004.67
8	954.345
9	922.658
10	901.253

```
Limit[λPa[n], n → ∞]
```

820.14

Brackett series

```
Nmax = 100; Nmin = 5; K = λBr[Nmin] - λBr[Nmax];
H1 = (λBr[Nmin] + λBr[Nmax]) / 2;
Graphics[
 {Line[{{λBr[Nmax], 0}, {λBr[Nmin], 0}}],
  Line[{{λBr[Nmax], K}, {λBr[Nmin], K}}],
  Hue[0.6], Thick,
  Table[Line[{{λBr[n], 0}, {λBr[n], K}}],
   {n, Nmin, 100}],
  Text[Style["Brackett series", Black, 15],
   {H1, K / 2}]}, Axes → {True, False},
 Ticks → {Range[1500, 4500, 500]},
 AxesLabel → {"λ(nm)"}]
```



```
Prepend[Table[{n, λBr[n] }, {n, 5, 10}],
  {"n", "λBr[nm]"}] // TableForm
```

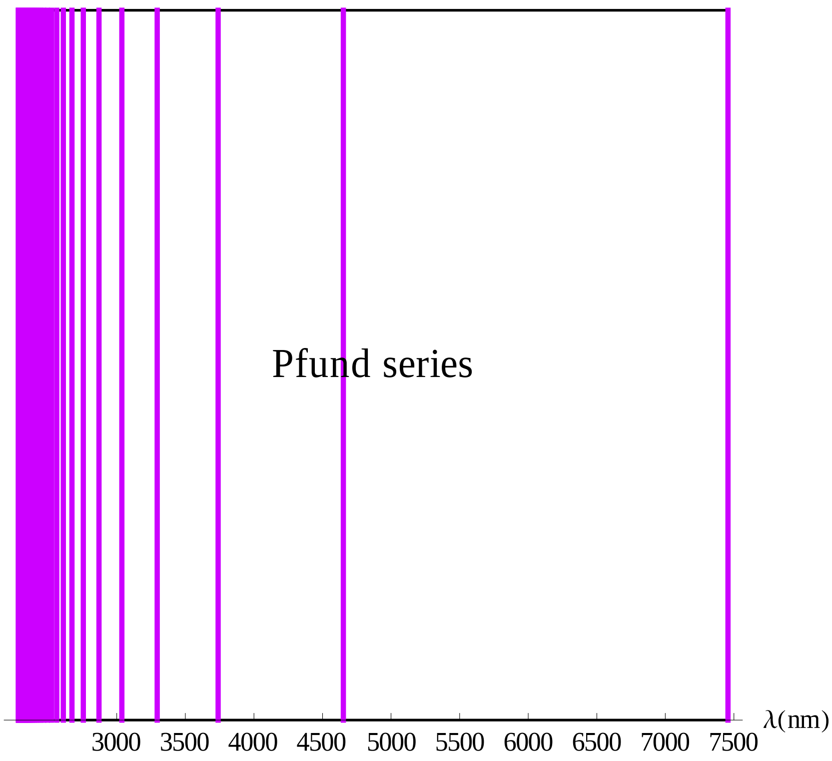
n	λBr[nm]
5	4050.08
6	2624.45
7	2164.95
8	1944.04
9	1816.93
10	1735.75

```
Limit[λBr[n], n → ∞]
```

1458.03

Pfund series

```
Nmax = 100; Nmin = 6; K = λPf[Nmin] - λPf[Nmax];
H1 = (λPf[Nmin] + λPf[Nmax]) / 2;
Graphics[
 {Line[{{λPf[Nmax], 0}, {λPf[Nmin], 0}}],
  Line[{{λPf[Nmax], K}, {λPf[Nmin], K}}],
  Hue[0.8], Thick,
  Table[Line[{{λPf[n], 0}, {λPf[n], K}}],
   {n, Nmin, 100}],
  Text[Style["Pfund series", Black, 15],
   {H1, K / 2}]}, Axes → {True, False},
 Ticks → {Range[3000, 7500, 500]},
 AxesLabel → {"λ(nm)"}]
```



```
Prepend[Table[{n, λPf[n] }, {n, 6, 10}],
  {"n", "λPf[nm]"}] // TableForm
```

n	λPf[nm]
6	7455.82
7	4651.26
8	3738.53
9	3295.21
10	3037.56

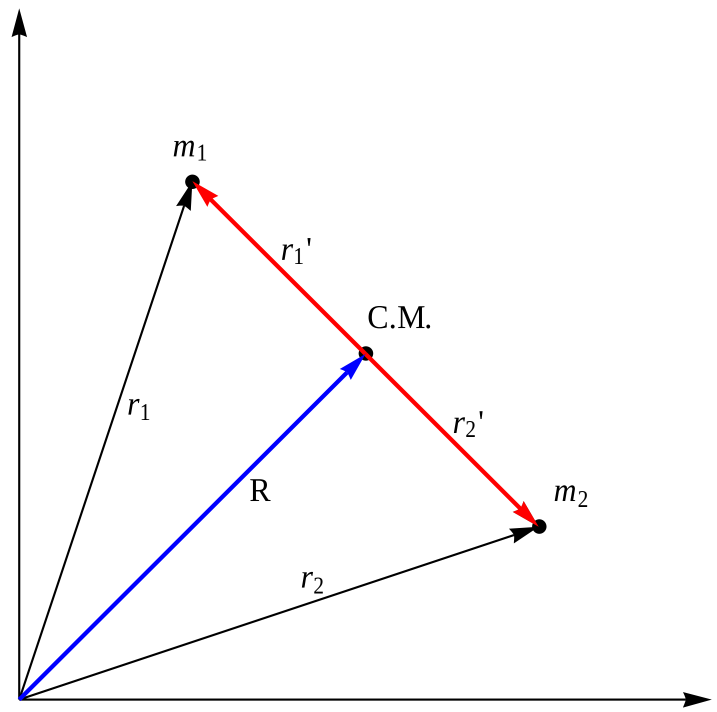
```
Limit[λPf[n], n → ∞]
```

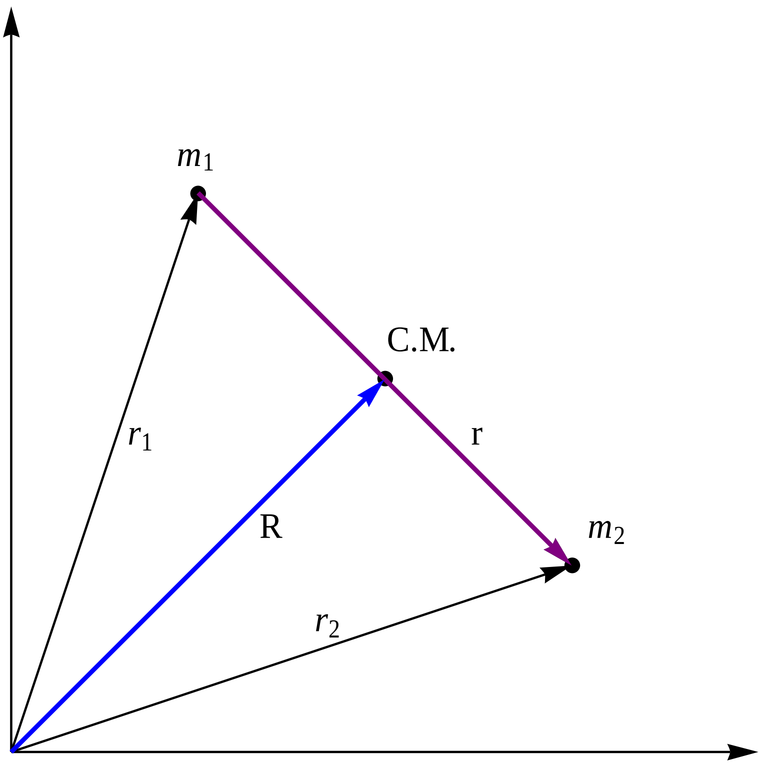
2278.17

3. Reduction of the equivalent one body problem

Problem of two bodies moving under the influence of a mutual central force.

We discuss this problem using the Lagrangian.





We consider a system of two mass points m1 and m1, where the only forces are due to a interaction potential. The Lagrange equation is given by

$$L = K - V = \frac{1}{2} m_1 \mathbf{r}_1{}^2 + \frac{1}{2} m_2 \mathbf{r}_2{}^2 - V(\mathbf{r})$$

From Fig. we have

$$\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1 = \mathbf{r}_2' - \mathbf{r}_1'$$

The center of mass

$$\mathbf{R} = \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2}$$

Here we note that

$$\mathbf{r}_1 = \mathbf{R} + \mathbf{r}_1', \qquad \mathbf{r}_2 = \mathbf{R} + \mathbf{r}_2'$$

Then

$$(m_1 + m_2)\mathbf{R} = m_1(\mathbf{R} + \mathbf{r}_1') + m_2(\mathbf{R} + \mathbf{r}_2')$$

or

$$m_1\mathbf{r}_1' + m_2\mathbf{r}_2' = 0$$

From two equations,

$$m_1\mathbf{r}_1' + m_2\mathbf{r}_2' = 0, \qquad \mathbf{r}_2' - \mathbf{r}_1' = \mathbf{r}$$

we get

$$\mathbf{r}_1' = -\frac{m_2}{m_1 + m_2}\mathbf{r}, \qquad \mathbf{r}_2' = \frac{m_1}{m_1 + m_2}\mathbf{r}$$

and

$$\mathbf{r}_1 = \mathbf{R} + \mathbf{r}_1' = \mathbf{R} - \frac{m_2}{m_1 + m_2}\mathbf{r}, \qquad \mathbf{r}_1 = \mathbf{R} + \mathbf{r}_2' = \mathbf{R} + \frac{m_1}{m_1 + m_2}\mathbf{r}$$

Then the kinetic energy is rewritten as

$$\begin{aligned}
K &= \frac{1}{2}m_1\dot{\mathbf{r}}_1^2 + \frac{1}{2}m_2\dot{\mathbf{r}}_2^2 \\
&= \frac{1}{2}m_1(\dot{\mathbf{R}} - \frac{m_2}{m_1 + m_2}\dot{\mathbf{r}})^2 + \frac{1}{2}m_2(\dot{\mathbf{R}} + \frac{m_1}{m_1 + m_2}\dot{\mathbf{r}})^2 \\
&= \frac{1}{2}m_1[\dot{\mathbf{R}}^2 - \frac{2m_2}{m_1 + m_2}\mathbf{R}\cdot\dot{\mathbf{r}} + (\frac{m_2}{m_1 + m_2}\dot{\mathbf{r}})^2] \\
&\quad + \frac{1}{2}m_2[\dot{\mathbf{R}}^2 + \frac{2m_1}{m_1 + m_2}\mathbf{R}\cdot\dot{\mathbf{r}} + (\frac{m_1}{m_1 + m_2}\dot{\mathbf{r}})^2] \\
&= \frac{1}{2}(m_1 + m_2)\dot{\mathbf{R}}^2 + \frac{1}{2}[m_1(\frac{m_2}{m_1 + m_2})^2\dot{\mathbf{r}}^2 + m_2(\frac{m_1}{m_1 + m_2})^2\dot{\mathbf{r}}^2 \\
&= \frac{1}{2}(m_1 + m_2)\dot{\mathbf{R}}^2 + \frac{1}{2}[\frac{m_1 m_2^2 + m_1^2 m_2}{(m_1 + m_2)^2}]\dot{\mathbf{r}}^2 \\
&= \frac{1}{2}(m_1 + m_2)\dot{\mathbf{R}}^2 + \frac{1}{2}\frac{m_1 m_2}{(m_1 + m_2)}\dot{\mathbf{r}}^2
\end{aligned}$$

The Lagrangian of this system does not contain a given co-ordinate R, then R is said to be a cyclic.

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{R}}}\right) - \frac{\partial L}{\partial \mathbf{R}} = 0,$$

or

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{R}}}\right) = 0$$

since

$$\frac{\partial L}{\partial \mathbf{R}} = 0$$

Then we have

$$(m_1 + m_2)\dot{\mathbf{R}} = const$$

The center of mass is either at rest or moving uniformly. We meryly drop the first term from the Lagrangian. Here we define a reduced mass such that

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

or

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

The Lagragian

$$L = \frac{1}{2}\mu \dot{\mathbf{r}}^2 - V(\mathbf{r})$$

Thus the central force motion of two bodies about their C.M. can always be reduced to an equivalent one-body problem.

4. Bohr model of electron with reduced mass

We now consider the effect of the reduced mass on the formula of the Bohr model. The reduced mass μ is defined as

$$\mu = \frac{mM}{m + M}$$

where m is the mass of electron and M is the mass of proton. In the formula for the Bohr model, m is replaced by the reduced mass.

$$v_n = \frac{1}{n}\frac{e^2}{4\pi\varepsilon_0\hbar}$$

$$r_n = 4\pi\varepsilon_0\frac{n^2\hbar^2}{\mu e^2} = n^2 r_B$$

where

$$r_B = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2} = a_0\frac{m}{\mu}$$

Then the total energy is obtained by

$$E_n = -\frac{e^2}{8\pi\varepsilon_0 n^2 r_B} = -\frac{E_0}{n^2}\frac{\mu}{m} = -\frac{\mu e^4}{2(4\pi\varepsilon_0)^2 n^2\hbar^2}$$

where

$$E_0 = \frac{e^2}{8\pi\varepsilon_0 a_0} = \frac{e^2}{8\pi\varepsilon_0\frac{4\pi\varepsilon_0\hbar^2}{me^2}} = \frac{me^4}{2(4\pi\varepsilon_0)^2\hbar^2}$$

E_0 =13.6057 eV

The Rydberg constant is given by

$$R = \frac{E_0}{hc}\frac{\mu}{m} = \frac{E_0}{hc}\frac{1}{m}\frac{mM}{m+M} = \frac{E_0}{hc}\frac{M}{m+M} = \frac{E_0}{hc}\frac{1}{1+\frac{m}{M}}$$

4. Effect of charge *Ze* of nucleus

We show the formula when the charge of nucleus is Ze.

$$\frac{mv^2 r}{mvr} = \frac{Ze^2}{n\hbar(4\pi\varepsilon_0)},$$

or

$$v = \frac{1}{n}\frac{Ze^2}{4\pi\varepsilon_0\hbar}$$

Then we get

$$m\left(\frac{Ze^2}{n4\pi\varepsilon_0\hbar}\right)^2 r = \frac{Ze^2}{4\pi\varepsilon_0},$$

or

$$r_n = \frac{4\pi\varepsilon_0}{Z}\frac{n^2\hbar^2}{me^2} = \frac{n^2 a_0}{Z}$$

where

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 5.29177 \text{ x } 10^{-11} \text{ m} = 0.529177 \text{ Å}$$

Then the total energy is obtained by

$$E_n = -\frac{Ze^2}{8\pi\varepsilon_0 r_n} - \frac{Z^2 e^2}{8\pi\varepsilon_0 n^2 a_0} = -Z^2\frac{E_0}{n^2}$$

where

$$E_0 = \frac{e^2}{8\pi\varepsilon_0 a_0} = \frac{e^2}{8\pi\varepsilon_0 \frac{4\pi\varepsilon_0\hbar^2}{me^2}} = \frac{me^4}{2(4\pi\varepsilon_0)^2\hbar^2}$$

E_0 =13.6057 eV