

ATOMIC REACTIONS PACKAGE INTRODUCTION

01/05/2026 (V1.0)

B. Michel Döhring
E-Mail: micheld.93@gmail.com

Contents		10 Dielectronic Recombination (DR)	5
1 Introduction	1	11 Trielectronic Recombination (TR)	7
2 Version History	2	12 Trielectronic Capture (TC)	7
2.1 Version 1.0 (01.05.2026)	2	13 Resonant elastic scattering (RES)	8
3 Repository and Contact	2	14 Resonant excitation (RE)	8
4 Future ideas	3	15 Inner-shell electron removal and subsequent autoionisation via Auger (ISERAA)	9
4.1 Atomic reactions	3	16 Bohr atomic model	10
4.2 Bohr's atomic model	3	16.1 Usage in <i>AtomicReactions</i>	10
5 Empty place holder	3	16.2 Derivation of the Bohr Radius . .	11
6 Direct ionisation (DI)	4	16.3 Derivation of the Bohr Energy Levels	12
7 Excitation auto-ionisation (EA)	4	References	14
8 REDA and READI	5		
9 Ionisation auto-ionisation (IA)	5		

1 Introduction

This package is named "*AtomicReactions*". In atomic physics, the electron shells and their behaviour under collisions with electrons or photons are the scope of the research field. This package provides commands to create term schemes for basic atomic reactions of the electron shells. For electron-impact single ionisation a number of specific reactions are possible which are:

- Direct ionisation (DI)
- Excitation auto-ionisation (EA)

- Resonant double auto-ionisation (REDA)
- Resonant auto-double-ionisation (READI)

For double and multiple ionisation dedicated processes are possible like *ionisation auto-ionisation*. Since the shell of an atom is a concept one can illustrate nicely by a picture, the goal of this package is to provide TikZ [1] drawings of those processes mentioned above. They are based on the drawings of Müller [2] to illustrate the behaviour of the electrons in the shell for the different reactions possible.

This package also provides a classical illustration for the atomic model by Niels Bohr [3], which shows the shells and electrons in dependence of occupation and chemical element. The approach here is easy. In case you want to have more customisation options, please try the package `bohr` by Clemens Niederberger [4]. Both packages can be used at the same time.

The *AtomicReactions*-package can be loaded with the following command:

```
\usepackage{atomicreactions}
```

2 Version History

All changes are collected in this chapter.

2.1 Version 1.0 (01.05.2026)

- first commit
- DI, EA, REDA, READI, IA implementation
- DR, TR, TC, RES, ISERAA

3 Repository and Contact

The repository/this package is available on GitHub and through CTAN [5] and TeXLive [6]. You will find it here:

- <https://www.ctan.org/pkg/apreax>
- <https://github.com/micheld93/APreax-Latex/>

If you have suggestions, problems or you only want to say "Hi", then contact me at micheld.93@gmail.com.

4 Future ideas

4.1 Atomic reactions

- additional reactions (multiple ionisation by electron impact)
- Auger including double auger etc.
- Photoionisation

4.2 Bohr's atomic model

- Term shematics
- Adjust colors (shells)
- Shell labels
- Bohr and orbitals (s,p,d,f) support
- Nucleus with p/n distribution with Z scaling
- Highlight the valence electrons
- automatic scaling of shell radius ($r \propto n^2$)
- Isotope support

5 Empty place holder

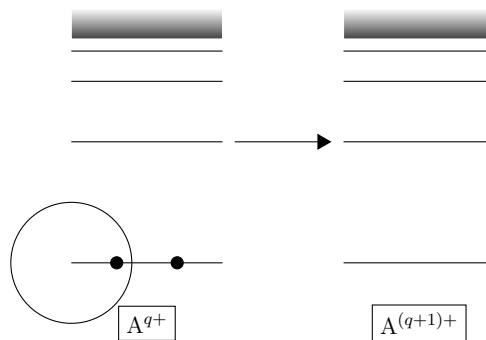


Figure 1: Just an empty place holder.

```
\begin{figure}[htp]
\centering
\atomEMPTY
\caption[Skizze zur direkte Einfachionisation]{Skizze zur direkte Einfachionisa
\label{pic:prozess:EMPTY-einfach}
\end{figure}
```

6 Direct ionisation (DI)

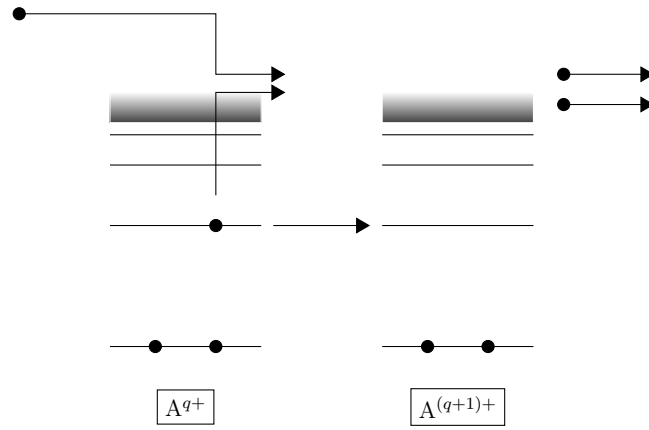


Figure 2: Direct ionisation.

```
\begin{figure}[htp]
\centering
\atomDI
\caption[Direct ionisation]{Direct ionisation.}
\label{pic:prozess:DI-single}
\end{figure}
```

7 Excitation auto-ionisation (EA)

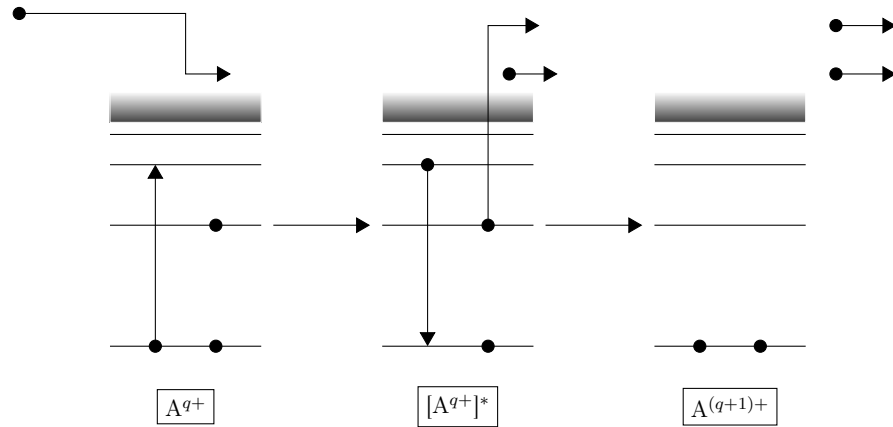


Figure 3: Excitation auto-ionisation (EA).

```
\begin{figure}[htp]
\centering
\atomEA
\caption[Excitation auto-ionisation (EA)]{Excitation auto-ionisation (EA).}
\label{pic:prozess:EA-single}
\end{figure}
```

8 REDA and READI

READI is the abbreviation for: Resonant Excitation in Autoionizing Double Ionization REDA is the the abbreviation for: Resonant Excitation Double Autoionization

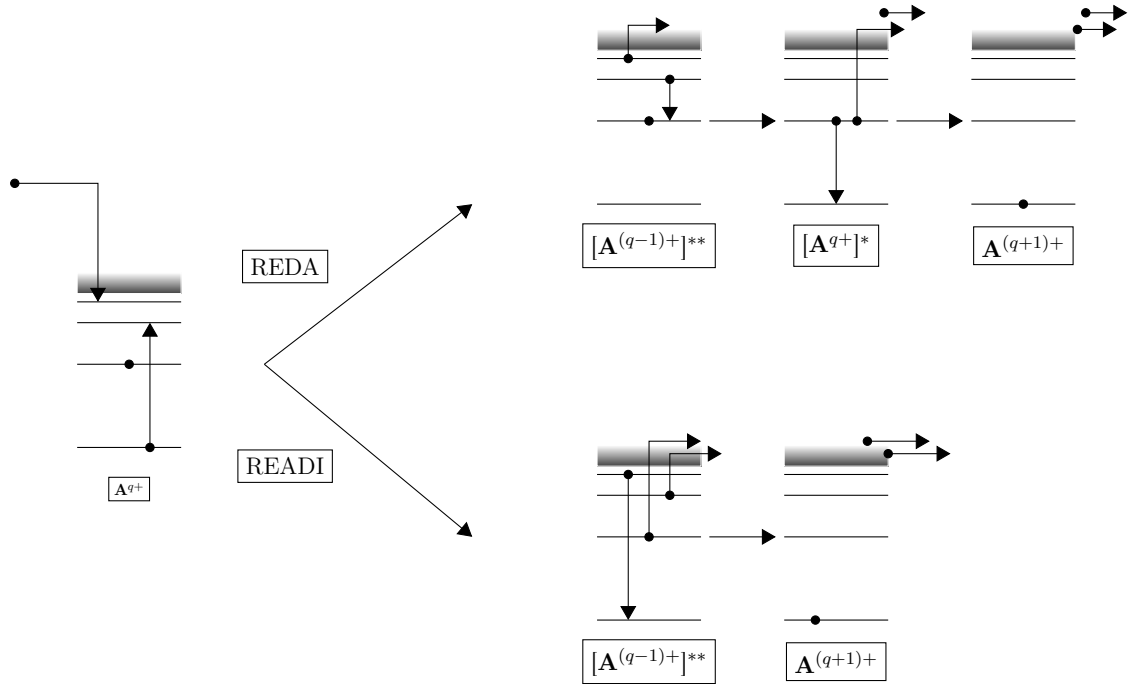


Figure 4: REDA and READI.

```
\begin{figure}[htp]
\centering
\atomREDA[0.55][1.5]
\caption[REDA and READI]{REDA and READI.}
\label{pic:prozess:REDA-READI}
\end{figure}
```

9 Ionisation auto-ionisation (IA)

```
\begin{figure}[htp]
\centering
\atomIA
\caption[Ionisation auto-ionisation (IA)]{Ionisation auto-ionisation (IA).}
\label{pic:prozess:IA}
\end{figure}
```

10 Dielectronic Recombination (DR)

```
\begin{figure}[htp]
\centering
```

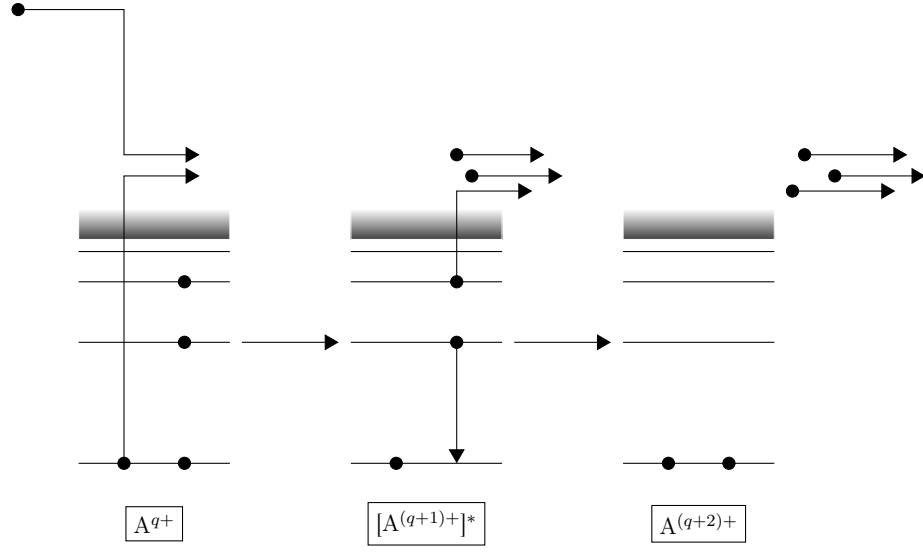


Figure 5: Ionisation auto-ionisation (IA).

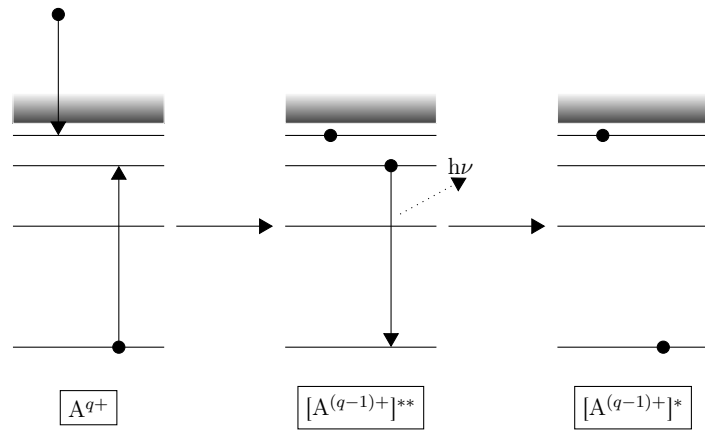


Figure 6: Dielectronic Recombination (DR).

```

\atomIA
\caption[Dielectronic Recombination (DR)]{Dielectronic Recombination (DR).}
\label{pic:prozess:DR}
\end{figure}

```

11 Trielectronic Recombination (TR)

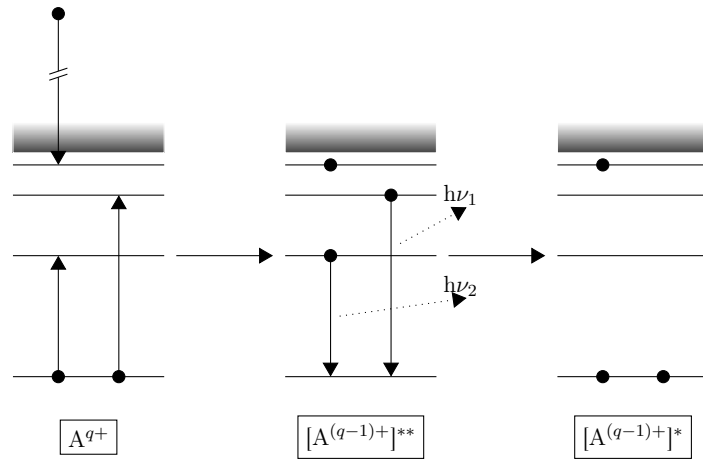


Figure 7: Trielectronic Recombination (TR).

```

\begin{figure}[htp]
\centering
\atomTR
\caption[Trielectronic Recombination (TR)]{Trielectronic Recombination (TR).}
\label{pic:prozess:TR}
\end{figure}

```

12 Trielectronic Capture (TC)

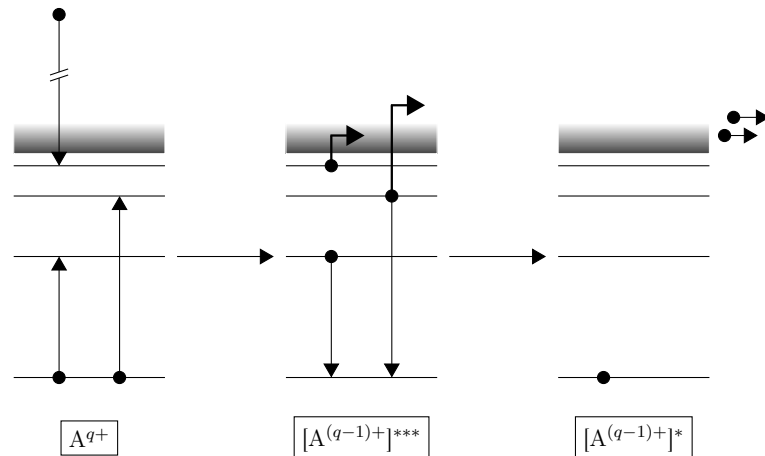


Figure 8: Trielectronic Capture (TC).

```

\begin{figure}[htp]
\centering
\atomTC
\caption[Trielectronic Capture (TC)]{Trielectronic Capture (TC).}
\label{pic:prozess:TC}
\end{figure}

```

13 Resonant elastic scattering (RES)

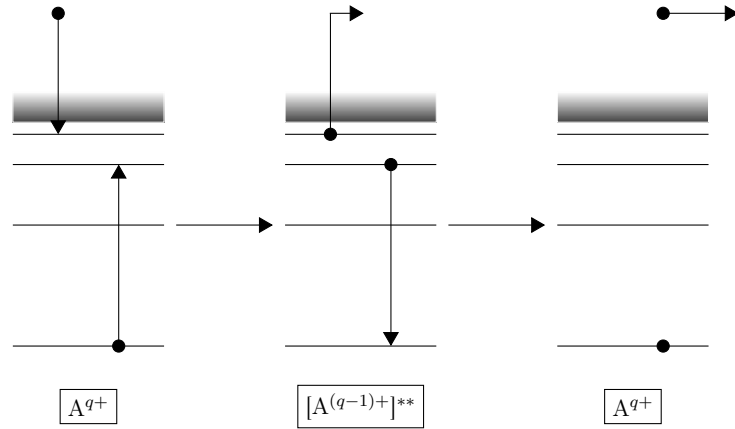


Figure 9: Resonant elastic scattering (RES)n.

```

\begin{figure}[htp]
\centering
\atomRES
\caption[Resonant elastic scattering (RES)]{Resonant elastic scattering (RES)n.}
\label{pic:prozess:RES}
\end{figure}

```

14 Resonant excitation (RE)

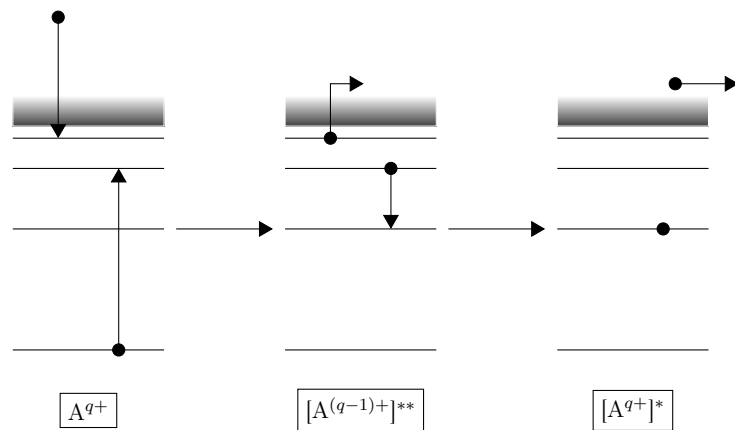


Figure 10: Resonant excitation (RE).


```

\begin{figure}[htp]
\centering
\atomRE
\caption[Resonant excitation (RE)]{Resonant excitation (RE).}
\label{pic:prozess:RE}
\end{figure}

```

15 Inner-shell electron removal and subsequent autoionisation via Auger (ISERAA)

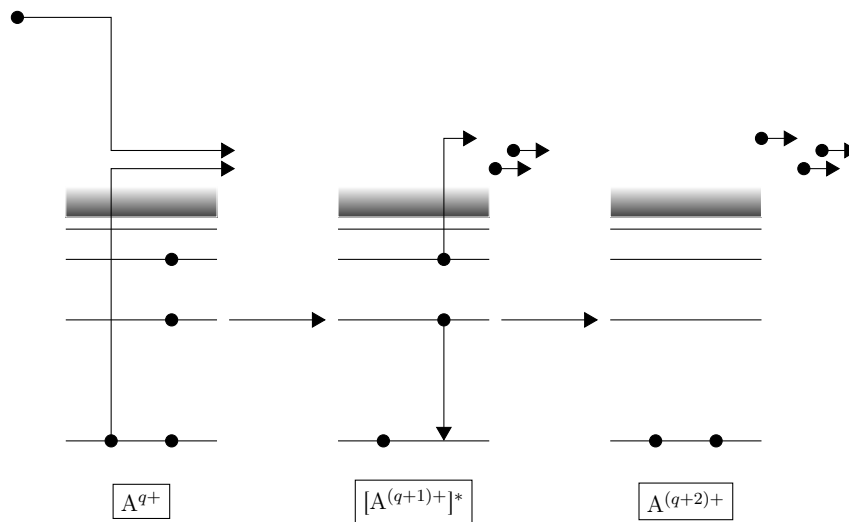


Figure 11: Inner-shell electron removal and subsequent autoionisation via Auger (ISERAA).

```

\begin{figure}[htp]
\centering
\atomISHAU
\caption[ISERAA]{ISERAA}
\label{pic:prozess:ISERAA}
\end{figure}

```

16 Bohr atomic model

In 1913, Nils Bohr published his groundbreaking paper on the later called "Bohr atomic model" [3], where he used a classical approach with an added discrete, quantum mechanical treatment of the angular momentum. The problem was that classical electromagnetism suggested that accelerating charged particles like electrons in orbits leads to a radiative energy release. Subsequently, this would lead to electrons collapsing into the nucleus. Since there were no evidence for this, new physics must be hidden. Bohr proposed that electrons reside in stable, specific orbits (discrete) without radiating. Energy can only be radiated when an electron jumps between these permitted orbits (quantum leap). Furthermore, he quantised the angular momentum L of an electron to integer multiples of $\hbar = \frac{h}{2\pi}$ to: $L = m \cdot v \cdot r = \frac{n \cdot h}{2\pi}$, where n is the main quantum number. The model succeeded to predict the spectral lines of hydrogen (Rydberg formula) later and established the concept of atomic shells occupied by electrons ($n = 1, 2, 3, \dots$). As a short reminder how to derive the Bohr formula, see the last chapter 16.2 If you just want to see how to use the Bohr model in this package, go to chapter 16.1.

16.1 Usage in *AtomicReactions*

AtomicReactions provides the following command:

```
\bohrModel{Xe}{5}{2,8,18,18,3}
```

which creates this nice TikZ picture:

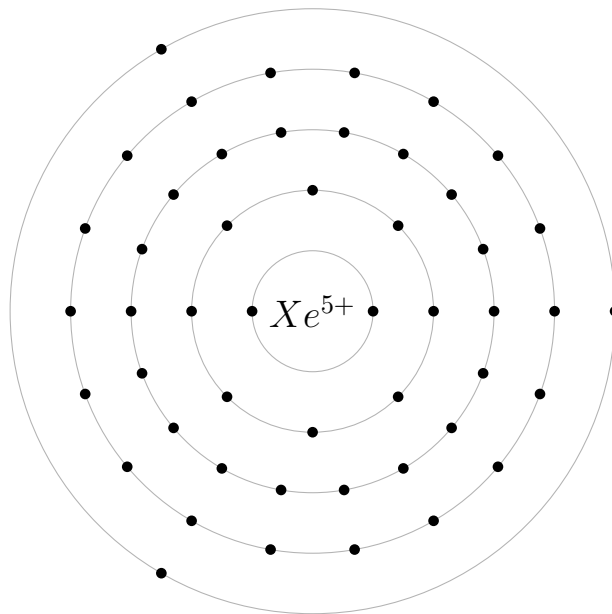


Figure 12: Bohr model for Xe^{5+}

The command has the following structure:

```
\bohrModel{Element-Name}{Charge}{K,L,M,N,O,P,Q}
```

As "Element-name" you can type whatever you want, but the most sense gives the common abbreviations from the periodic table. Charge needs to be filled, even if you have an atom

instead of an ion. K, L, M, N, O, P, Q indicates the shell name and needs to be filled with numbers. The numbers are the electrons in the specific shell. With this, you can also create pictures where an inner shell excitation is possible because inner-shell electrons are missing.

Table 1: Number of electrons in each shell

Shell name	Subshell name	Subshell max. electrons	Shell max. electrons	Subshell label	Angular momentum ℓ
K	1s	2	2	s	0
L	2s	2	8	p	1
	2p	6			
M	3s	2	18	d	2
	3p	6			
	3d	10			
	4s	2			
N	4p	6	32	g	4
	4d	10			
	4f	14			
	5s	2			
O	5p	6	50		
	5d	10			
	5f	14			
	5g	18			

16.2 Derivation of the Bohr Radius

For an electron orbiting a nucleus, the Coulomb force provides the centripetal force:

$$\frac{m_e v^2}{r} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2} \Leftrightarrow m_e v^2 = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \quad (1)$$

With Bohr's momentum quantization (Quantum mechanics!): $L = m_e v r = \frac{n\hbar}{2\pi} = n\hbar$

$$v = \frac{n\hbar}{m_e r} \quad (2)$$

Substitute the velocity in the force equation:

$$m_e \left(\frac{n\hbar}{m_e r} \right)^2 = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \quad (3)$$

Expand this:

$$\frac{n^2 \hbar^2}{m_e r^2} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \Leftrightarrow \frac{n^2 \hbar^2}{m_e} = \frac{1}{4\pi\epsilon_0} e^2 r \quad (4)$$

Solve for r :

$$r_n = \frac{4\pi\epsilon_0 n^2 \hbar^2}{m_e e^2} = n^2 a_0 \quad (5)$$

where the Bohr radius a_0 is

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} \approx 5.29 \times 10^{-11} \text{ m} \quad (6)$$

16.3 Derivation of the Bohr Energy Levels

The kinetic energy is

$$T = \frac{1}{2} m_e v^2 \quad (7)$$

From the force equation (Eq. 8):

$$m_e v^2 = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \quad (8)$$

Thus:

$$T = \frac{1}{2} \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \quad (9)$$

The electrostatic potential energy is

$$V = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \quad (10)$$

Total Energy

The total energy is

$$E = T + V \quad (11)$$

Substitute T and V :

$$E = \frac{1}{2} \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \quad (12)$$

$$E = -\frac{1}{2} \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \quad (13)$$

Now substitute r_n :

$$r_n = \frac{4\pi\epsilon_0 n^2 \hbar^2}{m_e e^2} \quad (14)$$

Then we get the following with substitution of r_n :

$$E_n = -\frac{1}{2} \frac{1}{4\pi\epsilon_0} \frac{e^2}{r_n} \Rightarrow E_n = -\frac{m_e e^4}{2(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{n^2} \quad (15)$$

Thus the Bohr energy levels for hydrogen are:

$$E_n = -\frac{13.6}{n^2} \text{ eV} \quad (16)$$

References

- [1] Christian Feuersänger and Till Tantau: *Tikz*. CTAN, 2015. <https://www.ctan.org/pkg/pgf>, visited on 13.02.2016, time: 12:43.
- [2] A. Müller: *Electron-ion collisions: Fundamental processes in the focus of applied research*. In *Advances in atomic, molecular and optical physics, Vol. 55*, pages 293–417. Academic Press, 2008.
- [3] N. Bohr: *On the Constitution of Atoms and Molecules*. Philosophical Magazine and Journal of Science, Series 6, 26(151):293–417, 1913.
- [4] Clemens Niederberger: *bohr*. CTAN, 2015. <https://www.ctan.org/pkg/bohr>, visited on 13.02.2026, time: 12:45.
- [5] CTAN: *Ctan*, 2016. <https://www.ctan.org>, visited on 13.02.2016, time: 12:44.
- [6] TeXLive: *Texlive*, 2016. <https://www.tug.org/texlive/>, visited on 13.02.2016, time: 12:45.