

FundamentalConstants.py

Physical Constants for Atomic Physics

CODATA Values and Atomic Parameters

ElecSus Library Documentation

Abstract

This document provides comprehensive documentation for `FundamentalConstants.py`, which defines the fundamental physical constants required for atomic spectroscopy calculations. These constants form the foundation for computing Zeeman shifts, hyperfine structure, and optical transitions in alkali atoms.

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1 Theoretical Foundation

1.1 Fundamental Constants in Atomic Physics

Axiom 1 (CODATA Standards). *Physical constants used in precision atomic physics calculations must conform to CODATA recommended values to ensure reproducibility and accuracy across different implementations.*

Definition 1 (Bohr Magneton). *The Bohr magneton is the natural unit of magnetic moment for an electron:*

$$\mu_B = \frac{e\hbar}{2m_e} \approx 9.274 \times 10^{-24} \text{ J/T} \quad (1)$$

Definition 2 (Electron g-factor). *The electron spin g-factor relates the magnetic moment to the spin angular momentum:*

$$\vec{\mu}_s = -g_s \frac{\mu_B}{\hbar} \vec{S} \quad (2)$$

where $g_s \approx 2.002319$ (including QED corrections).

Theorem 1 (Zeeman Energy). *The magnetic interaction energy for an electron in field \vec{B} is:*

$$H_Z = -\vec{\mu} \cdot \vec{B} = \mu_B(g_L L_z + g_S S_z)B \quad (3)$$

where $g_L = 1$ for orbital and $g_S \approx 2$ for spin contributions.

1.2 Atomic Units and Conversions

Definition 3 (Bohr Radius). *The characteristic length scale of atomic physics:*

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \approx 5.292 \times 10^{-11} \text{ m} \quad (4)$$

Definition 4 (Atomic Mass Unit). *The unified atomic mass unit:*

$$1 \text{ amu} = \frac{m(^{12}\text{C})}{12} \approx 1.661 \times 10^{-27} \text{ kg} \quad (5)$$

2 Line-by-Line Code Analysis

2.1 Module Imports

```
1 from numpy import pi, sqrt
2 from scipy.constants import physical_constants, epsilon_0, hbar, c, e,
```

Import mathematical functions and CODATA physical constants from SciPy.

2.2 Electron Spin

```
1 S=0.5 #Electron spin
```

$$S = \frac{1}{2} \quad (6)$$

Fundamental quantum number for electron spin. All alkali atoms have a single valence electron with $S = 1/2$.

2.3 Electron g-factor

```
1 gs = -physical_constants['electron_g_factor'][0]
```

$$g_s = -g_e \approx 2.002319 \quad (7)$$

The negative sign convention ensures proper orientation of magnetic moment relative to spin. The CODATA value includes QED corrections.

2.4 Bohr Magneton

```
1 muB=physical_constants['Bohr_magneton'][0]
```

$$\mu_B = \frac{e\hbar}{2m_e} = 9.274009994 \times 10^{-24} \text{ J/T} \quad (8)$$

Natural unit for atomic magnetic moments, essential for Zeeman effect calculations.

2.5 Boltzmann Constant

```
1 kB=physical_constants['Boltzmann_constant'][0]
```

$$k_B = 1.380649 \times 10^{-23} \text{ J/K} \quad (9)$$

Relates temperature to thermal energy, crucial for Doppler broadening calculations.

2.6 Atomic Mass Unit

```
1 amu=physical_constants['atomic_mass_constant'][0]
```

$$1 \text{ amu} = 1.66053906660 \times 10^{-27} \text{ kg} \quad (10)$$

Used to convert atomic masses to SI units for velocity calculations.

2.7 Vacuum Permittivity

```
1 e0=epsilon_0 #Permittivity of free space
```

$$\epsilon_0 = 8.8541878128 \times 10^{-12} \text{ F/m} \quad (11)$$

Appears in dipole matrix element calculations and field-matter interactions.

2.8 Bohr Radius

```
1 a0=physical_constants['Bohr_radius'][0]
```

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = 5.29177210903 \times 10^{-11} \text{ m} \quad (12)$$

Characteristic atomic length scale, defines the size of electronic wavefunctions.

3 Physical Applications

3.1 Zeeman Effect Calculations

The magnetic field interaction uses μ_B and g_s :

$$\Delta E = \mu_B B(m_L g_L + m_S g_S + m_I g_I) \quad (13)$$

3.2 Doppler Width

Temperature-dependent line broadening uses k_B and atomic mass:

$$\Delta\nu_D = \nu_0 \sqrt{\frac{8k_B T \ln 2}{mc^2}} \quad (14)$$

3.3 Dipole Matrix Elements

The transition dipole moment involves a_0 and e :

$$d = e\langle\psi_f|\vec{r}|\psi_i\rangle \sim e \cdot a_0 \quad (15)$$

4 Summary

This module provides the essential physical constants for atomic physics calculations:

1. $S = 1/2$: Electron spin quantum number
2. $g_s \approx 2$: Electron spin g-factor
3. μ_B : Bohr magneton for magnetic interactions
4. k_B : Boltzmann constant for thermal effects
5. ϵ_0, a_0 : Electromagnetic and atomic length scales
6. amu: Mass unit for velocity/Doppler calculations

These constants are imported by other modules in the ElecSus package for computing atomic spectra.