AtomConstants.py

Atomic and Transition Constants

Spectroscopic Data for Alkali Atoms

ElecSus Library Documentation

Abstract

This document provides comprehensive documentation for `AtomConstants.py`, which contains all spectroscopic constants for alkali atoms supported by the ElecSus library. These include nuclear spins, hyperfine constants, transition wavelengths, and natural linewidths essential for calculating atomic spectra.

Contents

1 Theoretical Foundation

1.1 Atomic Structure Parameters

Definition 1 (Nuclear Spin)**.** *The nuclear spin I determines the hyperfine structure:*

$$F = |I - J|, |I - J| + 1, \ldots, I + J \tag{1}$$

giving $(2\min(I, J) + 1)$ hyperfine levels for each fine structure state.

Definition 2 (Magnetic Dipole Hyperfine Constant)**.** *The A coefficient characterizes the $\vec{I} \cdot \vec{J}$ interaction:*

$$A = \frac{\mu_0 g_I \mu_N \mu_B}{4\pi} \frac{1}{IJ} \langle r^{-3} \rangle \tag{2}$$

Definition 3 (Electric Quadrupole Hyperfine Constant)**.** *The B coefficient (for $I \geq 1$, $J \geq 1$):*

$$B = eQ\langle \frac{\partial^2 V}{\partial z^2} \rangle_0 \tag{3}$$

where Q is the nuclear quadrupole moment.

Theorem 1 (Hyperfine Energy Levels)**.** *The hyperfine energy is:*

$$E_{HFS} = \frac{A \cdot K}{2} + B \frac{\frac{3}{2}K(K+1) - 2I(I+1)J(J+1)}{4I(2I-1)J(2J-1)} \tag{4}$$

where $K = F(F+1) - I(I+1) - J(J+1)$.

1.2 Transition Properties

Definition 4 (Natural Linewidth)**.** *The spontaneous decay rate determines the natural linewidth:*

$$\Gamma = \frac{\omega_0^3 |\langle e|d|g\rangle|^2}{3\pi\epsilon_0 \hbar c^3} \tag{5}$$

Definition 5 (Dipole Matrix Element)**.** *The transition dipole strength:*

$$d = \sqrt{\frac{3\epsilon_0 \hbar \Gamma \lambda^3}{8\pi}} \tag{6}$$

2 Atomic Species Classes

2.1 Rubidium-85

```python
class Rb85:
    """Constants relating to the rubidium-85 atom"""
    I  = 2.5          #Nuclear spin
    As = 1011.910813 #Ground state hyperfine constant in units of MHz
    gI = -0.00029364 #nuclear spin g-factor
    mass = 84.911789732*amu
    FS = 7.123e6 # Fine-structure splitting
```

Parameter	Value	Units
I	$5/2$	–
A_s	1011.91	MHz
g_I	-2.9364×10^{-4}	–
mass	84.91	amu
Δ_{FS}	7.123	THz

Table 1: ^{85}Rb atomic constants

2.2 Rubidium-87

```
class Rb87:
    """Constants relating to the rubidium-87 atom"""
    I  = 1.5
    As = 3417.341305452145
    gI = -0.0009951414
    mass = 86.909180520*amu
    FS = 7.123e6
```

^{87}Rb has smaller nuclear spin ($I = 3/2$) but larger hyperfine constant than ^{85}Rb.

2.3 Cesium-133

```
class Cs:
    """Constants relating to the caesium-133 atom"""
    I  = 3.5
    As = 2298.1579425
    gI = -0.00039885395
    mass = 132.905451931*amu
    FS = 351725718.50 - 335116048.807
```

The Cs ground state hyperfine splitting (9.19 GHz) defines the SI second.

2.4 Potassium Isotopes

```
class K39:
    I  = 1.5
    As = 230.8598601
    # ...

class K40:
    I  = 4.0
    As = -285.7308  # Negative due to nuclear structure
    # ...

class K41:
    I  = 1.5
    As = 127.0069352
    # ...
```

^{40}K is notable for having negative hyperfine constant and large nuclear spin.

2.5 Sodium-23

```
class Na:
    I  = 1.5
    As = 885.81306440
    gI = -0.00080461080
    mass = 22.9897692807*amu
```

3 Transition Classes

3.1 D-Line Transitions

Definition 6 (D1 and D2 Lines)**.** *The D-lines are transitions from the ground $nS_{1/2}$ state:*

$$D1: \quad nS_{1/2} \to nP_{1/2} \tag{7}$$

$$D2: \quad nS_{1/2} \to nP_{3/2} \tag{8}$$

3.2 Rubidium D-Lines

```
class RbD1Transition:
    wavelength=794.978969380e-9
    wavevectorMagnitude=2.0*pi/wavelength
    NatGamma=5.746  # MHz
    dipoleStrength=3.0*sqrt(e0*hbar*(2.0*NatGamma*(10.0**6))*(
        wavelength**3)/(8.0*pi))
    v0=377107407.299e6  # Hz

class RbD2Transition:
    wavelength=780.2413272e-9
    NatGamma=6.065
    v0=384230426.6e6
```

Transition	λ (nm)	ν_0 (THz)	Γ (MHz)
Rb D1	794.98	377.11	5.75
Rb D2	780.24	384.23	6.07

Table 2: Rubidium D-line parameters

3.3 Cesium D-Lines

```
class CsD1Transition:
    wavelength=894.59295986e-9
    NatGamma=4.584
    v0=335116048.807e6

class CsD2Transition:
    wavelength=852.34727582e-9
    NatGamma=5.225
    v0=351725718.50e6
```

4 Isotope-Transition Classes

4.1 Excited State Hyperfine Constants

```
class Rb87_D2:
    Ap = 84.7185       # MHz
    Bp = 12.4965       # MHz
    IsotopeShift = -56.361   # MHz
```

Theorem 2 (Isotope Shift)**.** *The isotope shift arises from:*

$$\Delta E_{IS} = \Delta E_{mass} + \Delta E_{field} \tag{9}$$

where mass shift is due to nuclear recoil and field shift is due to finite nuclear size.

4.2 Complete Parameter Tables

Isotope	Transition	A_p (MHz)	B_p (MHz)	IS (MHz)
^{85}Rb	D1	120.64	0	21.62
^{85}Rb	D2	25.04	26.01	21.73
^{87}Rb	D1	406.15	0	−56.08
^{87}Rb	D2	84.72	12.50	−56.36
^{133}Cs	D1	291.92	0	0
^{133}Cs	D2	50.29	−0.49	0

Table 3: Excited state hyperfine parameters

5 Usage Notes

5.1 Dipole Strength Formula

The code computes the reduced dipole matrix element:

```
dipoleStrength=3.0*sqrt(e0*hbar*(2.0*NatGamma*(10.0**6))*(wavelength
    **3)/(8.0*pi))
```

This follows from inverting the spontaneous emission rate formula.

5.2 Transitions Dictionary

```
transitions = {'RbD1':RbD1Transition, 'RbD2':RbD2Transition,
               'CsD1':CsD1Transition, 'CsD2':CsD2Transition,
               # ...
              }
```

Enables programmatic access to transition properties by name.

6 Summary

The `AtomConstants.py` module provides:

1. Atomic species classes: Nuclear spin, hyperfine constants, mass

2. Transition classes: Wavelength, linewidth, dipole strength

3. Isotope-transition classes: Excited state parameters, isotope shifts

4. Convenience dictionary for programmatic access

Supported species: Rb-85, Rb-87, Cs-133, K-39, K-40, K-41, Na-23, IdealAtom.
All constants are in SI units except hyperfine constants (MHz) and masses (amu).