## Contents

1. **Contents**  
   1.1 Installation instructions ................................................................. 3  
   1.2 Getting started with ARC ................................................................. 5  
   1.3 Detailed documentation of functions ............................................... 5  
   1.4 How to contribute to the project ..................................................... 43

2. **Package structure**  

3. **Indices and tables**  

4. **Credits**  

Python Module Index  

Index
ARC (Alkali Rydberg Calculator) is a package of routines written in Python, using object-oriented programming (OOP) to make modular, reusable and extendable collection of routines and data for performing useful calculations of single atom and two-atom properties, like level diagrams, interactions and transition strengths for alkali metal atoms.
1.1 Installation instructions

1.1.1 Prerequisite: Python

Install Python and packages for scientific computing in Python (scipy, numpy, matplotlib). The package is tested and works with both Python 2.7 and Python 3.6. We recommend installing Python distributions that comes with Numpy that is connected to the optimized numeric libraries like ATLAS. One such distribution is Anaconda, that provides ATLAS support and optimized math kernel.

1.1.2 Recommended installation: via Python pip

Users can simply install the package from command line:

```
pip install ARC-Alkali-Rydberg-Calculator
```

This finishes installation. This should work on all operating systems (Linux, OSX, Windows) with Python 2.7 or Python 3.6. Note this is a new feature for Windows, so Windows users should contact developers if unexpected errors occur. Below we describe some old (legacy) installation methods.

1.1.3 Download the ARC library/package

Download latest release for your operating system, unzip the archive and set the folder somewhere within the Python package search path or directly in your project directory. Simply import and use the module:

```
from arc import *
# write your code that uses ARC then.
```

It is important that package is stored somewhere where user has write permissions, so that it can update the databases with atomic properties. This is the end of the standard installation for majority of the users.

1.1.4 Installation of the package globally with setup.py

This is tested on Linux so far
Do this only if you have Linux/UNIX (as it is tested on it) and you are sure that you don’t want to change underlying ARC code. Make sure you have C compiler and python development headers installed. To compile and install for local user ARC call from terminal:

```
python setup.py build
python setup.py install
```

Databases that have to be changed with new values will be locally copied from package data location to ~/.arc-data folder when arc is used for the first time.

### 1.1.5 Compiling C extension

If you do need to compile C extension yourself, this is how to do it without installing globally the package (as in the previous section “Installation of the package globally with setup.py”). Optimized version of the Numerov is provided as the C code `arc_c_extensions.c`. **You don’t need to perform this step** of manual compilation of that code if you followed recommended installation instruction by downloading precompiled binary distribution for the latest release. Note that path to arc directory **should not contain spaces** in order to setupc.py script to work.

**For Windows users**

If precompiled binaries don’t work, please contact developers. Compiling Numpy C extensions on Windows is a bit complicated due to use of C89 standard (instead of C99). Procedure is the following. One needs to use MSVC compiler in order to compile Numpy extension for Python 2.7 under Windows. For other Python versions (3.5) find correct compiler here. After installation of the compiler, find in Start menu “Visual C++ 2008 32-bit Command Prompt” (for 32-bit Python) or “Visual C++ 2008 64-bit Command Prompt” (for 64-bit Python). Set the following variables set in the command prompt environment:

```
SET DISTUTILS_USE_SDK=1
SET MSSdk=1
python setupc.py build_ext --inplace
```

This should build C Numpy extension (implementing Numerov integration) under Windows. We recommend, however, using pre-build binaries available on the release page.

**For Linux users**

Download and install GNU C compiler. Then with terminal open, navigate to arc folder where setupc.py file is located execute:

```
python setupc.py build_ext --inplace
```

**For Mac users**

Download and install GNU C compiler. Then with terminal open, navigate to arc folder where setupc.py file is located execute:

```
python setupc.py build_ext --inplace
```

**Slow alternative: Numerov implemented in pure Python**

Alternative solution, if you don’t want to compile anything, is to use pure Python implementation of the Numerov, provided in the package. This is done by passing `cpp_numerov = False` flag whenever atoms are initialized, e.g:

```
atom = Rubidium(cpp_numerov=False)
```

This is not recommended option for complex calculations, since it will run much more slowly then optimized C version, but is fine if you need just a few numbers.

**Finally...**

That is all, enjoy using ARC package. Check **IPython notebook with examples** to see some ideas where to start.
1.2 Getting started with ARC

1.2.1 IPython notebook with examples

Rydberg atoms - a primer introduces Rydberg atoms and ARC package, and is a good starting point to learn how to use ARC to get relevant information about alkali metal Rydberg atoms. Notebook can also be downloaded in .ipython format here, and can be interactively then modified and used in a Jupyter.

1.2.2 On demand examples from online Atom calculator

You can try using the package without installing anything on your computer. Simply point your web browser from your computer, tablet or phone to atomcalc.jqc.org.uk and use ARC online.

Online version also generates the correct code necessary for answering the questions you ask, which can be downloaded and used as a starting point for running the package locally on your computer.

1.2.3 Frequently asked questions (FAQ)

If you have a question how to do a common calculation, we recommend checking above mentioned Rydberg atoms - a primer IPython notebook. For general questions about the package usage check here:

1. How to save calculation (or matrix) for later use?

Calculations of pair-state interactions PairStateInteractions and Stark maps StarkMap can be easily saved at any point by calling alkali_atom_functions.saveCalculation. This can be loaded later by using alkali_atom_functions.loadSavedCalculation and calculation can be continued from that point.

2. How to export results?

If you want to export results e.g. for analysis and plotting in other programs, you can use calculations_atom_pairstate.PairStateInteractions.exportData and calculations_atom_single.StarkMap.exportData to export results of Stark map and Pair-state interaction calculations in .csv format. See documentation of corresponding functions for more details.

3. Calculation is not outputting anything? How long does it take for calculation to finish?

Most of the functions have progressOutput and debugOutput as an optional parameter (by default set to False) - check documentation of individual functions for details. We recommend setting at least progressOutput=True so that you have minimum output about the status of calculations. This often displays percentage of the current calculation that is finished, that you can use to estimate total time. Setting debugOutput=True outputs even more verbose output, like states in the selected basis, and individual coupling strengths etc.

1.3 Detailed documentation of functions

1.3.1 Alkali atom functions

Overview

Classes and global methods
Alkali Atom

AlkaliAtom([preferQuantumDefects, cpp_numrov])

Implements general calculations for alkali atoms.

NumerovBack(innerLimit, outerLimit, kfun, ...) Full Python implementation of Numerov integration

saveCalculation(calculation, fileName) Saves calculation for future use.

loadSavedCalculation(fileName) Loads previously saved calculation.

printState(n, l, j) Prints state spectroscopic label for numeric n, l, s label of the state

printStateString(n, l, j) Returns state spectroscopic label for numeric n, l, s label of the state

AlkaliAtom Methods

AlkaliAtom.getDipoleMatrixElement(n1, l1, ...) Dipole matrix element \(\langle n_1l_1j_1m_j_1 | \vec{r} | n_2l_2j_2m_j_2 \rangle\) in units of \(a_0e\)

AlkaliAtom.getTransitionWavelength(n1, l1, ...) Calculated transition wavelength (in vacuum) in m.

AlkaliAtom.getTransitionFrequency(n1, l1, ...) Calculated transition frequency in Hz

AlkaliAtom.getRabiFrequency(n1, l1, j1, mj1, ...) Returns a Rabi frequency for resonantly driven atom in a center of TEM00 mode of a driving field.

AlkaliAtom.getRabiFrequency2(n1, l1, j1, ...) Returns a Rabi frequency for resonant excitation with a given electric field amplitude.

AlkaliAtom.getStateLifetime(n, l, j[, ...]) Returns the lifetime of the state (in s)

AlkaliAtom.getTransitionRate(n1, l1, j1, n2, ...) Transition rate due to coupling to vacuum modes (black body included)

AlkaliAtom.getReducedMatrixElementJ_asymmetric(n1, ...) Reduced matrix element in \(J\) basis, defined in asymmetric notation.

AlkaliAtom.getReducedMatrixElementJ(n1, l1, ...) Reduced matrix element in \(J\) basis (symmetric notation)

AlkaliAtom.getReducedMatrixElementL(n1, l1, ...) Reduced matrix element in \(L\) basis (symmetric notation)

AlkaliAtom.getRadialMatrixElement(n1, l1, ...) Radial part of the dipole matrix element

AlkaliAtom.getQuadrupoleMatrixElement(n1, l1, ...) Radial part of the quadrupole matrix element

AlkaliAtom.getPressure(temperature) Vapour pressure (in Pa) at given temperature

AlkaliAtom.getNumberDensity(temperature) Atom number density at given temperature

AlkaliAtom.getAverageInteratomicSpacing(temperature) Returns average interatomic spacing in atomic vapour

AlkaliAtom.corePotential(l, r) core potential felt by valence electron

AlkaliAtom.effectiveCharge(l, r) effective charge of the core felt by valence electron

AlkaliAtom.potential(l, s, j, r) returns total potential that electron feels

AlkaliAtom.radialWavefunction(l, s, j, ...) Radial part of electron wavefunction

AlkaliAtom.getEnergy(n, l, j) Energy of the level relative to the ionisation level (in eV)

AlkaliAtom.getZeemanEnergyShift(l, j, mj[, ...]) Returns linear (paramagnetic) Zeeman shift.

AlkaliAtom.getQuantumDefect(n, l, j) Quantum defect of the level.

AlkaliAtom.getC6term(n, l, j, n1, l1, j1, ...) C6 interaction term for the given two pair-states

AlkaliAtom.getC3term(n, l, j, n1, l1, j1, ...) C3 interaction term for the given two pair-states

AlkaliAtom.getEnergyDefect(n, l, j, n1, l1, ...) Energy defect for the given two pair-states (one of the state has two atoms in the same state)

AlkaliAtom.getEnergyDefect2(n, l, j, nn, ll, ...) Energy defect for the given two pair-states

Continued on next page
Alkali Rydberg Calculator (ARC) Documentation, Release 2.0.6

Table 2 – continued from previous page

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlkaliAtom.updateDipoleMatrixElements()</td>
<td>Updates the file with pre-calculated dipole matrix elements.</td>
</tr>
<tr>
<td>AlkaliAtom.getRadialCoupling(n, l, j, n1, l1, j1)</td>
<td>Returns radial part of the coupling between two states (dipole and quadrupole interactions only)</td>
</tr>
<tr>
<td>AlkaliAtom.getAverageSpeed(temperature)</td>
<td>Average (mean) speed at a given temperature</td>
</tr>
<tr>
<td>AlkaliAtom.getLiteratureDME(n1, l1, j1, n2, ...)</td>
<td>Returns literature information on requested transition.</td>
</tr>
</tbody>
</table>

**Detailed documentation**

Implements general single-atom calculations

This module calculates single (isolated) atom properties of all alkali metals in general. For example, it calculates dipole matrix elements, quadrupole matrix elements, etc. Also, some helpful general functions are here, e.g. for saving and loading calculations (single-atom and pair-state based), printing state labels etc.

```python
class arc.alkali_atom_functions.AlkaliAtom(preferQuantumDefects=True, cpp_numerov=True)
```

Implements general calculations for alkali atoms.

This abstract class implements general calculations methods.

**Parameters**

- `preferQuantumDefects (bool)` – Use quantum defects for energy level calculations. If False, uses NIST ASD values where available. If True, uses quantum defects for energy calculations for principal quantum numbers equal or above `minQuantumDefectN` which is specified for each element separately. For principal quantum numbers below this value, NIST ASD values are used, since quantum defects don’t reproduce well low-lying states. Default is True.

- `cpp_numerov (bool)` – should the wavefunction be calculated with Numerov algorithm implemented in C++; if False, it uses pure Python implementation that is much slower. Default is True.

```
Z = 0.0
Atomic number

a1 = [0]
Model potential parameters fitted from experimental observations for different l (electron angular momentum)

a2 = [0]
Model potential parameters fitted from experimental observations for different l (electron angular momentum)

a3 = [0]
Model potential parameters fitted from experimental observations for different l (electron angular momentum)

a4 = [0]
Model potential parameters fitted from experimental observations for different l (electron angular momentum)

abundance = 1.0
relative isotope abundance

alphaC = 0.0
Core polarizability

corePotential(l, r)
core potential felt by valence electron
```

1.3. Detailed documentation of functions
For more details about derivation of model potential see Ref. 2.

**Parameters**
- \( l \) (int) – orbital angular momentum
- \( r \) (float) – distance from the nucleus (in a.u.)

**Returns** core potential felt by valence electron (in a.u. ???)

**Return type** float

**References**

cpp_numerov = True

swich - should the wavefunction be calculated with Numerov algorithm implemented in C++

dipoleMatrixElementFile = ''
location of hard-disk stored dipole matrix elements

effectiveCharge\((l,r)\)
effective charge of the core felt by valence electron

For more details about derivation of model potential see Ref. 2.

**Parameters**
- \( l \) (int) – orbital angular momentum
- \( r \) (float) – distance from the nucleus (in a.u.)

**Returns** effective charge (in a.u.)

**Return type** float

elementName = 'elementName'
Human-readable element name

extraLevels = []
levels that are for smaller principal quantum number \( n \) than ground level, but are above in energy due to angular part

getAddressAverageInteratomicSpacing\((temperature)\)
Returns average interatomic spacing in atomic vapour

See calculation of basic properties example snippet.

**Parameters** temperature (float) – temperature of the atomic vapour

**Returns** average interatomic spacing in m

**Return type** float

getAddressAverageSpeed\((temperature)\)
Average (mean) speed at a given temperature

**Parameters** temperature (float) – temperature (K)

**Returns** mean speed (m/s)

**Return type** float

getAddressC3term\((n, l, j, n1, l1, j1, n2, l2, j2)\)
C3 interaction term for the given two pair-states

Calculates \( C_3 \) interaction term for \(|n,l,j,n,l,j\rangle \leftrightarrow |n_1,l_1,j_1,n_2,l_2,j_2\rangle\)

**Parameters**
- \( n \) (int) – principal quantum number

---

• \(l\) (int) – orbital angular momentum
• \(j\) (float) – total angular momentum
• \(n_1\) (int) – principal quantum number
• \(l_1\) (int) – orbital angular momentum
• \(j_1\) (float) – total angular momentum
• \(n_2\) (int) – principal quantum number
• \(l_2\) (int) – orbital angular momentum
• \(j_2\) (float) – total angular momentum

Returns \(C_3 = \frac{\langle n,l,j \mid e_r \mid n_1,l_1,j_1 \rangle \langle n,l,j \mid e_r \mid n_2,l_2,j_2 \rangle}{4\pi \varepsilon_0} (\text{Hz m}^3)\).

Return type float
getc6term\((n, l, j, n_1, l_1, j_1, n_2, l_2, j_2)\)
C6 interaction term for the given two pair-states

Calculates \(C_6\) interaction term for \(|n,l,j,n,l,j\rangle \leftrightarrow |n_1,l_1,j_1,n_2,l_2,j_2\rangle\). For details of calculation see Ref.\(^3\).

Parameters
• \(n\) (int) – principal quantum number
• \(l\) (int) – orbital angular momentum
• \(j\) (float) – total angular momentum
• \(n_1\) (int) – principal quantum number
• \(l_1\) (int) – orbital angular momentum
• \(j_1\) (float) – total angular momentum
• \(n_2\) (int) – principal quantum number
• \(l_2\) (int) – orbital angular momentum
• \(j_2\) (float) – total angular momentum

Returns \(C_6 = \frac{1}{4\pi \varepsilon_0} \frac{\left| \langle n,l,j \mid e_r \mid n_1,l_1,j_1 \rangle \rangle^2 \langle n,l,j \mid e_r \mid n_2,l_2,j_2 \rangle \rangle^2}{E(n_1,l_1,j_1,n_2,l_2,j_2) - E(n,l,j,n,l,j)} (\text{Hz m}^6)\).

Return type float

Example

We can reproduce values from Ref.\(^3\) for C3 coupling to particular channels. Taking for example channels described by the Eq. (50a-c) we can get the values:

```python
from arc import *

channels = [[[70,0,0.5, 70, 1,1.5, 69,1, 1.5],
             [70,0,0.5, 70, 1,1.5, 69,1, 0.5],
             [70,0,0.5, 69, 1,1.5, 70,1, 0.5],
             [70,0,0.5, 70, 1,0.5, 69,1, 0.5]]

print(" = = = Caesium = = =")
atom = Caesium()
for channel in channels:
    print("%.0f GHz (mu m)^6" % (atom.getC6term(*channel) / C_h * 1.e27
       \) →

(continues on next page)


1.3. Detailed documentation of functions
\begin{verbatim}
print("\n--- Rubidium ----")
atom = Rubidium()
for channel in channels:
    print("%.0f GHz (\mu m)^6" % (atom.getC6term(*channel) / C_h * 1.e27))
\end{verbatim}

Returns:

--- Caesium ---
722 GHz (\mu m)^6
316 GHz (\mu m)^6
383 GHz (\mu m)^6
228 GHz (\mu m)^6
--- Rubidium ---
799 GHz (\mu m)^6
543 GHz (\mu m)^6
589 GHz (\mu m)^6
437 GHz (\mu m)^6

which is in good agreement with the values cited in the Ref.\(^3\). Small discrepancies for Caesium originate from slightly different quantum defects used in calculations.

References

\textbf{getDipoleMatrixElement}\((n1, l1, j1, mj1, n2, l2, j2, mj2, q)\)
Dipole matrix element \(\langle n_1 l_1 j_1 m_j | e r | n_2 l_2 j_2 m_j \rangle\) in units of \(a_0 e\)

Returns dipole matrix element \((a_0 e)\)

Return type \(\text{float}\)

Example

For example, calculation of \(5S_{1/2} m_j=-0.5 \rightarrow 5P_{3/2} m_j=-1.5\) transition dipole matrix element for laser driving \(\sigma^-\) transition:

\begin{verbatim}
from arc import *
atom = Rubidium()
# transition 5 S_{1/2} m_j=-0.5 -> 5 P_{3/2} m_j=-1.5 for laser
print(atom.getDipoleMatrixElement(5,0,0.5,-0.5,5,1,1.5,-1.5,-1))
\end{verbatim}

\textbf{getEnergy}\((n, l, j)\)
Energy of the level relative to the ionisation level \((\text{in eV})\)

Returned energies are with respect to the center of gravity of the hyperfine-split states. If \texttt{preferQuantumDefects} =\texttt{False} (set during initialization) program will try use NIST energy value, if such exists, falling back to energy calculation with quantum defects if the measured value doesn’t exist. For \texttt{preferQuantumDefects} =\texttt{True}, program will always calculate energies from quantum defects (useful for comparing quantum defect calculations with measured energy level values).

Parameters

\begin{itemize}
    \item \texttt{n (int)} – principal quantum number
    \item \texttt{l (int)} – orbital angular momentum
    \item \texttt{j (float)} – total angular momentum
\end{itemize}

Returns state energy \((\text{eV})\)
Return type  float

getEnergyDefect \( (n, l, j, n1, l1, j1, n2, l2, j2) \)
Energy defect for the given two pair-states (one of the state has two atoms in the same state)
Energy difference between the states \( E(n_1, l_1, j_1, n_2, l_2, j_2) - E(n, l, j, n, l, j) \)

Parameters

- \( n (int) \) – principal quantum number
- \( l (int) \) – orbital angular momentum
- \( j (float) \) – total angular momentum
- \( n1 (int) \) – principal quantum number
- \( l1 (int) \) – orbital angular momentum
- \( j1 (float) \) – total angular momentum
- \( n2 (int) \) – principal quantum number
- \( l2 (int) \) – orbital angular momentum
- \( j2 (float) \) – total angular momentum

Returns  energy defect (SI units: J)

Return type  float

getEnergyDefect2 \( (n, l, j, nn, ll, jj, n1, l1, j1, n2, l2, j2) \)
Energy defect for the given two pair-states
Energy difference between the states \( E(n_1, l_1, j_1, n_2, l_2, j_2) - E(n, l, j, nn, ll, jj) \)
See pair-state energy defects example snippet.

Parameters

- \( n (int) \) – principal quantum number
- \( l (int) \) – orbital angular momentum
- \( j (float) \) – total angular momentum
- \( nn (int) \) – principal quantum number
- \( ll (int) \) – orbital angular momentum
- \( jj (float) \) – total angular momentum
- \( n1 (int) \) – principal quantum number
- \( l1 (int) \) – orbital angular momentum
- \( j1 (float) \) – total angular momentum
- \( n2 (int) \) – principal quantum number
- \( l2 (int) \) – orbital angular momentum
- \( j2 (float) \) – total angular momentum

Returns  energy defect (SI units: J)

Return type  float

getLiteratureDME \( (n1, l1, j1, n2, l2, j2) \)
Returns literature information on requested transition.

Parameters

- \( n1, l1, j1 \) – one of the states we are coupling
- \( n2, l2, j2 \) – the other state to which we are coupling
Returns

hasLiteratureValue?, dme, referenceInformation

If Boolean value is True, a literature value for dipole matrix element was found and reduced DME in J basis is returned as the number. Third returned argument (array) contains additional information about the literature value in the following order [ typeOfSource, errorEstimate, comment, reference, reference DOI] upon success to find a literature value for dipole matrix element:

- typeOfSource=1 if the value is theoretical calculation; otherwise, if it is experimentally obtained value typeOfSource=0
- comment details where within the publication the value can be found
- errorEstimate is absolute error estimate
- reference is human-readable formatted reference
- reference DOI provides link to the publication.

Boolean value is False, followed by zero and an empty array if no literature value for dipole matrix element is found.

Return type  bool, float, [int, float, string, string, string]

Note:  The literature values are stored in /data folder in <element name>_literature_dme.csv files as a ; separated values. Each row in the file consists of one literature entry, that has information in the following order:

- n1
- l1
- j1
- n2
- l2
- j2
- dipole matrix element reduced l basis (a.u.)
- comment (e.g. where in the paper value appears?)
- value origin: 1 for theoretical; 0 for experimental values
- accuracy
- source (human readable formatted citation)
- doi number (e.g. 10.1103/RevModPhys.82.2313)

If there are several values for a given transition, program will output the value that has smallest error (under column accuracy). The list of values can be expanded - every time program runs this file is read and the list is parsed again for use in calculations.

getNumberDensity (temperature)
Atom number density at given temperature

See calculation of basic properties example snippet.

Parameters  temperature (float) – temperature in K

Returns  atom concentration in $1/m^3$

Return type  float

getPressure (temperature)
Vapour pressure (in Pa) at given temperature
Parameters **temperature** (`float`) – temperature in K

Returns vapour pressure in Pa

Return type `float`

`getQuadrupoleMatrixElement` \((n1, l1, j1, n2, l2, j2)\)
Radial part of the quadrupole matrix element

Calculates \(\int dr R_{n_1, l_1, j_1}(r) \cdot R_{n_1, l_1, j_1}(r) \cdot r^4\). See Quadrupole calculation example snippet.

Parameters
- `n1` (`int`) – principal quantum number of state 1
- `l1` (`int`) – orbital angular momentum of state 1
- `j1` (`float`) – total angular momentum of state 1
- `n2` (`int`) – principal quantum number of state 2
- `l2` (`int`) – orbital angular momentum of state 2
- `j2` (`float`) – total angular momentum of state 2

Returns quadrupole matrix element \(a_2^0 e\).

Return type `float`

`getQuantumDefect` \((n, l, j)\)
Quantum defect of the level.

For an example, see Rydberg energy levels example snippet.

Parameters
- `n` (`int`) – principal quantum number
- `l` (`int`) – orbital angular momentum
- `j` (`float`) – total angular momentum

Returns quantum defect

Return type `float`

`getRabiFrequency` \((n1, l1, j1, m_{j1}, n2, l2, j2, q, laserPower, laserWaist)\)
Returns a Rabi frequency for resonantly driven atom in a center of TEM00 mode of a driving field

Parameters
- `n1, l1, j1, m_{j1}` – state from which we are driving transition
- `n2, l2, j2` – state to which we are driving transition
- `q` – laser polarization (-1,0,1 correspond to \(\sigma^-, \pi \) and \(\sigma^+\) respectively)
- `laserPower` – laser power in units of W
- `laserWaist` – laser \(1/e^2\) waist (radius) in units of m

Returns Frequency in rad \(^{-1}\). If you want frequency in Hz, divide by returned value by \(2\pi\)

Return type `float`

`getRabiFrequency2` \((n1, l1, j1, m_{j1}, n2, l2, j2, q, electricFieldAmplitude)\)
Returns a Rabi frequency for resonant excitation with a given electric field amplitude

Parameters
- `n1, l1, j1, m_{j1}` – state from which we are driving transition
- `n2, l2, j2` – state to which we are driving transition
- `q` – laser polarization (-1,0,1 correspond to \(\sigma^-, \pi \) and \(\sigma^+\) respectively)
• **electricFieldAmplitude** – amplitude of electric field driving (V/m)

**Returns**  Frequency in rad $^{-1}$. If you want frequency in Hz, divide by returned value by $2\pi$

**Return type**  float

**getRadialCoupling** ($n, l, j, n1, l1, j1$)

Returns radial part of the coupling between two states (dipole and quadrupole interactions only)

**Parameters**

• $n1$ (*int*) – principal quantum number
• $l1$ (*int*) – orbital angular momentum
• $j1$ (*float*) – total angular momentum
• $n2$ (*int*) – principal quantum number
• $l2$ (*int*) – orbital angular momentum
• $j2$ (*float*) – total angular momentum

**Returns**  radial coupling strength (in a.u.), or zero for forbidden transitions in dipole and quadrupole approximation.

**Return type**  float

**getRadialMatrixElement** ($n1, l1, j1, n2, l2, j2$, *useLiterature=True*)

Radial part of the dipole matrix element

Calculates $\int dr\, R_{n1,l1,j1}(r) \cdot R_{n1,l1,j1}(r) \cdot r^3$.

**Parameters**

• $n1$ (*int*) – principal quantum number of state 1
• $l1$ (*int*) – orbital angular momentum of state 1
• $j1$ (*float*) – total angular momentum of state 1
• $n2$ (*int*) – principal quantum number of state 2
• $l2$ (*int*) – orbital angular momentum of state 2
• $j2$ (*float*) – total angular momentum of state 2

**Returns**  dipole matrix element ($a_0e$).

**Return type**  float

**getReducedMatrixElementJ** ($n1, l1, j1, n2, l2, j2$)

Reduced matrix element in $J$ basis (symmetric notation)

**Parameters**

• $n1$ (*int*) – principal quantum number of state 1
• $l1$ (*int*) – orbital angular momentum of state 1
• $j1$ (*float*) – total angular momentum of state 1
• $n2$ (*int*) – principal quantum number of state 2
• $l2$ (*int*) – orbital angular momentum of state 2
• $j2$ (*float*) – total angular momentum of state 2

**Returns**  reduced dipole matrix element in $J$ basis $\langle j||er||j'\rangle$ ($a_0e$).

**Return type**  float
getReducedMatrixElementJ_asymmetric(n1, l1, j1, n2, l2, j2)
Reduced matrix element in $J$ basis, defined in asymmetric notation.

Note that notation for symmetric and asymmetrically defined reduced matrix element is not consistent in the literature. For example, notation is used e.g. in Steck\(^1\) is precisely the opposite.

Note: Note that this notation is asymmetric: $(j||er||j') \neq (j'||er||j)$. Relation between the two notation is $(j||er||j') = \sqrt{2j + 1} (j||er||j)$. This function always returns value for transition from lower to higher energy state, independent of the order of states entered in the function call.

Parameters
- n1 (int) – principal quantum number of state 1
- l1 (int) – orbital angular momentum of state 1
- j1 (float) – total angular momentum of state 1
- n2 (int) – principal quantum number of state 2
- l2 (int) – orbital angular momentum of state 2
- j2 (float) – total angular momentum of state 2

Returns reduced dipole matrix element in Steck notation $(j||er||j') (a_0e)$.  
Return type float

getReducedMatrixElementL(n1, l1, j1, n2, l2, j2)
Reduced matrix element in $L$ basis (symmetric notation)

Parameters
- n1 (int) – principal quantum number of state 1
- l1 (int) – orbital angular momentum of state 1
- j1 (float) – total angular momentum of state 1
- n2 (int) – principal quantum number of state 2
- l2 (int) – orbital angular momentum of state 2
- j2 (float) – total angular momentum of state 2

Returns reduced dipole matrix element in $L$ basis $(l||er||l') (a_0e)$.  
Return type float

getStateLifetime(n, l, j, temperature=0, includeLevelsUpTo=0)
Returns the lifetime of the state (in s)

For non-zero temperatures, user must specify up to which principal quantum number levels, that is above the initial state, should be included in order to account for black-body induced transitions to higher lying states. See Rydberg lifetimes example snippet.

Parameters
- l, j (n,) – specifies state whose lifetime we are calculating
- temperature – optional. Temperature at which the atom environment is, measured in K. If this parameter is non-zero, user has to specify transitions up to which state (due to black-body decay) should be included in calculation.

---

\(^1\) Daniel A. Steck, “Cesium D Line Data,” (revision 2.0.1, 2 May 2008). http://steck.us/alkalidata
includeLevelsUpTo (int) – optional and not needed for atom lifetimes calculated at zero temperature. At non-zero temperatures, this specifies maximum principal quantum number of the state to which black-body induced transitions will be included. Minimal value of the parameter in that case is \( n + 1 \)

Returns State lifetime in units of s (seconds)

Return type float

See also:

getTransitionRate for calculating rates of individual transition rates between the two states

getTransitionFrequency \((n1, l1, j1, n2, l2, j2)\)

Calculated transition frequency in Hz

Returned values is given relative to the centre of gravity of the hyperfine-split states.

Parameters

- \( n1 \) (int) – principal quantum number of the state from which we are going
- \( l1 \) (int) – orbital angular momentum of the state from which we are going
- \( j1 \) (float) – total angular momentum of the state from which we are going
- \( n2 \) (int) – principal quantum number of the state to which we are going
- \( l2 \) (int) – orbital angular momentum of the state to which we are going
- \( j2 \) (float) – total angular momentum of the state to which we are going

Returns transition frequency (in Hz). If the returned value is negative, level from which we are going is above the level to which we are going.

Return type float

getTransitionRate \((n1, l1, j1, n2, l2, j2, temperature=0.0)\)

Transition rate due to coupling to vacuum modes (black body included)

Calculates transition rate from the first given state to the second given state \(|n1, l1, j1\rangle \rightarrow |n2, j2, j2\rangle\) at given temperature due to interaction with the vacuum field. For zero temperature this returns Einstein A coefficient. For details of calculation see Ref.\(^4\) and Ref.\(^5\). See Black-body induced population transfer example snippet.

Parameters

- \( n1 \) (int) – principal quantum number
- \( l1 \) (int) – orbital angular momentum
- \( j1 \) (float) – total angular momentum
- \( n2 \) (int) – principal quantum number
- \( l2 \) (int) – orbital angular momentum
- \( j2 \) (float) – total angular momentum
- \[temperature\] (float) – temperature in K

Returns transition rate in \( s^{-1} \) (SI)

Return type float


References

**getTransitionWavelength \((n1, l1, j1, n2, l2, j2)\)**
Calculated transition wavelength (in vacuum) in m.

Returned values is given relative to the centre of gravity of the hyperfine-split states.

**Parameters**
- \(n1\) (int) – principal quantum number of the state from which we are going
- \(l1\) (int) – orbital angular momentum of the state from which we are going
- \(j1\) (float) – total angular momentum of the state from which we are going
- \(n2\) (int) – principal quantum number of the state to which we are going
- \(l2\) (int) – orbital angular momentum of the state to which we are going
- \(j2\) (float) – total angular momentum of the state to which we are going

**Returns** transition wavelength (in m). If the returned value is negative, level from which we are going is above the level to which we are going.

**Return type** float

**getZeemanEnergyShift \((l, j, mj, magneticFieldBz)\)**
Returns linear (paramagnetic) Zeeman shift.

\[ \mathcal{H}_P = \frac{\mu B}{\hbar}(\hat{I}_z + g_S S_z) \]

**Returns** energy offset of the state (in J)

**Return type** float

**groundStateN = 0**
principal quantum number for the ground state

**levelDataFromNIST = ''**
location of stored NIST values of measured energy levels in eV

**literatureDMEfilename = ''**
Filename of the additional literature source values of dipole matrix elements.

These additional values should be saved as reduced dipole matrix elements in J basis.

**mass = 0.0**
atomic mass in kg

**minQuantumDefectN = 0**
minimal quantum number for which quantum defects can be used; uses measured energy levels otherwise

**potential \((l, s, j, r)\)**
returns total potential that electron feels

Total potential = core potential + Spin-Orbit interaction

**Parameters**
- \(l\) (int) – orbital angular momentum
- \(s\) (float) – spin angular momentum
- \(j\) (float) – total angular momentum
- \(r\) (float) – distance from the nucleus (in a.u.)

**Returns** potential (in a.u.)

**Return type** float
quadrupoleMatrixElementFile = ''
location of hard-disk stored dipole matrix elements

quantumDefect = [[[0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0]], [[0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0]]
Contains list of modified Rydberg-Ritz coefficients for calculating quantum defects for [[S_1/2, P_1/2, D_3/2, F_5/2], [S_3/2, P_3/2, D_5/2, F_7/2]].

radialWavefunction(l, s, j, stateEnergy, innerLimit, outerLimit, step)
Radial part of electron wavefunction

Calculates radial function with Numerov (from outside towards the core). Note that wavefunction might not be calculated all the way to the requested innerLimit if the divergence occurs before. In that case third returned argument gives nonzero value, corresponding to the first index in the array for which wavefunction was calculated. For quick example see Rydberg wavefunction calculation snippet.

Parameters
• l (int) – orbital angular momentum
• s (float) – spin angular momentum
• j (float) – total angular momentum
• stateEnergy (float) – state energy, relative to ionization threshold, should be given in atomic units (Hartree)
• innerLimit (float) – inner limit at which wavefunction is requested
• outerLimit (float) – outer limit at which wavefunction is requested
• step (float) – radial step for integration mesh (a.u.)

Returns
r
R(r) ∙ r

Return type List[float], List[float], int

Note: Radial wavefunction is not scaled to unity! This normalization condition means that we are using spherical harmonics which are normalized such that \( \int d\theta d\phi Y(l, ml)^* \times Y(l', ml') = \delta(l, l') \delta(ml, ml') \).

Note: Alternative calculation methods can be added here (potential package expansion).

rc = [0]
Model potential parameters fitted from experimental observations for different l (electron angular momentum)
scaledRydbergConstant = 0 in eV

updateDipoleMatrixElementsFile()
Updates the file with pre-calculated dipole matrix elements.
This function will add the file all the elements that have been calculated in the previous run, allowing quick access to them in the future calculations.

arc.alkali_atom_functions.NumerovBack(innerLimit, outerLimit, kfun, step, init1, init2)
Full Python implementation of Numerov integration

Calculates solution function \( rad(r) \) with discrete step in \( r \) size of \( step \), integrating from \( outerLimit \) towards the \( innerLimit \) (from outside, inwards) equation \( \frac{d^2 rad(r)}{dr^2} = kfun(r) \cdot rad(r) \).

Parameters
• `innerLimit (float)` – inner limit of integration
• `outerLimit (float)` – outer limit of integration
• `kfun (function(double))` – pointer to function used in equation (see longer explanation above)
• `step` – discrete step size for integration
• `init1 (float)` – initial value, `rad`('outerLimit'+ `step`)
• `init2 (float)` – initial value, `rad`('outerLimit' + `math: 2cdot step`)

Returns \( r \) (a.u), \( r \) \( \text{rad} \) (\( r \)),

Return type numpy array of float, numpy array of float, int

**Note:** Returned function is not normalized!

**Note:** If `AlkaliAtom.cpp_numerov` switch is set to True (default option), much faster C implementation of the algorithm will be used instead. That is recommended option. See documentation installation instructions for more details.

```python
arc.alkali_atom_functions.loadSavedCalculation(fileName)
```

Loads previously saved calculation.

    Loads calculations_atom_pairstate.PairStateInteractions and calculations_atom_single.StarkMap calculation instance from file named `filename` where it was previously saved with `saveCalculation`.

**Example**

See example for `saveCalculation`.

**Parameters** `fileName` – name of the file where calculation will be saved

**Returns** saved calculation

```python
arc.alkali_atom_functions.printState(n, l, j)
```

Prints state spectroscopic label for numeric \( n, l, s \) label of the state

**Parameters**

• `n (int)` – principal quantum number
• `l (int)` – orbital angular momentum
• `j (float)` – total angular momentum

```python
arc.alkali_atom_functions.printStateString(n, l, j)
```

Returns state spectroscopic label for numeric \( n, l, s \) label of the state

**Parameters**

• `n (int)` – principal quantum number
• `l (int)` – orbital angular momentum
• `j (float)` – total angular momentum

**Returns** label for the state in standard spectroscopic notation

**Return type** string

```python
arc.alkali_atom_functions.printStateStringLatex(n, l, j)
```

Returns latex code for spectroscopic label for numeric \( n, l, s \) label of the state
Parameters

- **n (int)** – principal quantum number
- **l (int)** – orbital angular momentum
- **j (float)** – total angular momentum

Returns label for the state in standard spectroscopic notation

Return type string

arc.alkali_atom_functions.saveCalculation(calculation, fileName)

Saves calculation for future use.

Saves calculations_atom_pairstate.PairStateInteractions and calculations_atom_single.StarkMap calculations in compact binary format in file named filename. It uses cPickle serialization library in Python, and also zips the final file.

Calculation can be retrieved and used with loadSavedCalculation

Parameters

- **calculation** – class instance of calculations (instance of calculations_atom_pairstate.PairStateInteractions or calculations_atom_single.StarkMap) to be saved.
- **fileName** – name of the file where calculation will be saved

Example

Let’s suppose that we did the part of the calculation_atom_pairstate.PairStateInteractions calculation that involves generation of the interaction matrix. After that we can save the full calculation in a single file:

```python
calc = PairStateInteractions(Rubidium(), 60, 0.5, 60, 0.5, 0.5, 0.5, 0.5)
calc.defineBasis(0, 0, 5, 5, 25.e9)
calc.diagonalise(np.linspace(0.5, 10.0, 200), 150)
saveCalculation(calc, "mySavedCalculation.pkl")
```

Then, at a later time, and even on the another machine, we can load that file and continue with calculation. We can for example explore the calculated level diagram:

```python
calc = loadSavedCalculation("mySavedCalculation.pkl")
calc.plotLevelDiagram()
calc.showPlot()
rvdw = calc.getVdwFromLevelDiagram(0.5, 14, minStateContribution=0.5, showPlot=True)
```

Or, we can do additional matrix diagonalization, in some new range, then and find C6 by fitting the obtained level diagram:

```python
calc = loadSavedCalculation("mySavedCalculation.pkl")
calc.diagonalise(np.linspace(3, 6.0, 200), 20)
calc.getC6fromLevelDiagram(3, 6.0, showPlot=True)
```

Note that for all loading of saved calculations we’ve been using function loadSavedCalculation.

Note: This doesn’t save results of plotLevelDiagram for the corresponding calculations. Call the plot function before calling showPlot function for the corresponding calculation.

arc.alkali_atom_functions.setup_data_folder()

Setup the data folder in the users home directory.
1.3.2 Alkali atom data

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<td>backward compatibility: before only one class for Potassium existed and it corresponded to Potassium 39</td>
<td>Properties of potassium 39 atoms</td>
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</table>

This module specifies properties of individual alkali metals.

If you want to change e.g. coefficients used for model potential, quantum defects, or other numerical values, this is the place to look at.

How to delete precalculated dipole/quadrupole matrix elements values and/or start a new database?

To delete precalculated values, simply delete files, whose names are stated in dipoleMatrixElementFile, quadrupoleMatrixElementFile and precalculatedDB variables for the corresponding atom type, from data/ folder. Alternatively, if you want to keep old values, but want to also start completely new calculation of dipole matrix elements (e.g. because you changed parameters of energy levels significantly or model potential parameters), simply set new values for dipoleMatrixElementFile, quadrupoleMatrixElementFile and precalculatedDB variables.

Note that by default isotopes of Rubidium and Potassium are sharing precalculated dipole and quadrupole matrix elements. This is because the small energy level differences typically don’t change this matrix elements within a typical accuracy.

Data sources

Module

class arc.alkali_atom_data.Caesium(preferQuantumDefects=True, cpp_numerov=True)

Properties of caesium atoms

\[
a_1 = [3.49546309, 4.69366096, 4.32466196, 3.01048361]
\]
model potential parameters from\(^1\)

\[
a_2 = [1.475338, 1.71398344, 1.61365288, 1.40000001]
\]
model potential parameters from\(^1\)

\[
a_3 = [-9.72143084, -24.6562428, -6.7012885, -3.20036138]
\]
model potential parameters from\(^1\)

\[
a_4 = [0.02629242, -0.09543125, -0.74095193, 0.00034538]
\]
model potential parameters from\(^1\)

alphaC = 15.644
model potential parameters from\textsuperscript{1}

extraLevels = \{[5, 2, 2.5], [5, 2, 1.5], [5, 3, 3.5], [5, 3, 2.5], [5, 4, 4.5], [5, 4, 3.5], [4, 3, 3.5], [4, 3, 2.5]\}
levels that are for smaller n than ground level, but are above in energy due to angular part

getPressure (temperature)
Pressure of atomic vapour at given temperature.
Uses equation and values from\textsuperscript{3}. Values from table 2. (accuracy +- 5%) are used for Cs in solid phase.
Values from table 3. (accuracy +-1 %) are used for Cs in liquid phase.

ionisationEnergy = 3.8939056946689456 (eV), Ref.\textsuperscript{9}

quantumDefect = \{[[4.04935665, 0.2377037, 0.255401, 0.00378, 0.25486, 0.0], [3.5915895, 0.360926, 0.41905, 0.64388, 0.0, 0.0], [3.03381565, 0.476537, 0.53475, 0.92483, 0.0, 0.0], [2.4760417, 0.710708, 0.77892, 1.35834, 0.0, 0.0], [1.91826775, 0.823777, 0.88199, 1.73832, 0.0, 0.0], [1.3604938, 0.823777, 0.88199, 1.73832, 0.0, 0.0], [0.80271985, 0.823777, 0.88199, 1.73832, 0.0, 0.0], [0.2449459, 0.823777, 0.88199, 1.73832, 0.0, 0.0]\}
quantum defects for $S_{1/2}$, $nP_{1/2}$, $D_{5/2}$, $F_{5/2}$ and $G_{7/2}$ are from\textsuperscript{1}, while quantum defects for $nP_{3/2}$ are from\textsuperscript{10}.

Note: $f_{7/2}$ quantum defects are PUT TO BE EXACTLY the same as $f_{5/2}$ (~10MHz difference?!)
a1 = [2.47718079, 3.45414648, 2.51909839, 2.51909839]
model potential parameters from^1

a2 = [1.84150932, 2.5515108, 2.4371245, 2.4371245]
model potential parameters from^1

a3 = [-0.02169712, -0.21646561, 0.32505524, 0.32505524]
model potential parameters from^1

a4 = [-0.11988362, -0.06990078, 0.1060243, 0.1060243]
model potential parameters from^1

abundance = 0.0759
source NIST, Atomic Weights and Isotopic Compositions^14

alphaC = 0.1923
model potential parameters from^1

getPressure(temperature)
Pressure of atomic vapour at given temperature.
Uses equation and values from^3. Values from table 3. (accuracy +-1 %) are used both for liquid and solid phase of Li.

mass = 9.988346384925222e-27
source NIST, Atomic Weights and Isotopic Compositions^14

quantumDefect = [[[0.3995101, 0.029, 0.0, 0.0, 0.0, 0.0], [0.0471835, -0.024, 0.0, 0.0, 0.0, 0.0], [0.002129, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0]], [[0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0]]]
quantum defects for nS and nP are from Ref.^8 . Quantum defects for D_1 and F_1 are from Ref.^11
(note that this defects in Ref.^11 are for Li7, differences are expected not be too big).

rc = [0.61340824, 0.61566441, 2.34126273, 2.34126273]
model potential parameters from^1

class arc.alkali_atom_data.Lithium7(preferQuantumDefects=True, cpp_numerov=True)
Properties of lithium 7 atoms

a1 = [2.47718079, 3.45414648, 2.51909839, 2.51909839]
model potential parameters from^1

a2 = [1.84150932, 2.5515108, 2.4371245, 2.4371245]
model potential parameters from^1

a3 = [-0.02169712, -0.21646561, 0.32505524, 0.32505524]
model potential parameters from^1

a4 = [-0.11988362, -0.06990078, 0.1060243, 0.1060243]
model potential parameters from^1

abundance = 0.9241
source NIST, Atomic Weights and Isotopic Compositions^14

alphaC = 0.1923
model potential parameters from^1

getPressure(temperature)
Pressure of atomic vapour at given temperature (in K).
Uses equation and values from^3. Values from table 3. (accuracy +-1 %) are used for both liquid and solid phase of Li.

ionisationEnergy = 5.391719
(eV) NIST Ref.^13.

---


mass = 1.1650347611248465e-26
source NIST, Atomic Weights and Isotopic Compositions

quantumDefect = [[[0.3995101, 0.029, 0.0, 0.0, 0.0, 0.0], [0.047178, -0.024, 0.0, 0.0, 0.0, 0.0], [0.002129, 0.052518, -0.1759, -0.8507, 0.0, 0.0], [-7.7e-05, 0.021856, -0.4211, 2.3891, 0.0, 0.0], [0.0, 0.0, 0.0, 0.0, 0.0, 0.0]]
quantum defects for nS and nP states are from Ref. 8. Quantum defects for D_j and F_j states are from 11.

rc = [0.61340824, 0.61566441, 2.34126273, 2.34126273]
model potential parameters from 1

class arc.alkali_atom_data.Potassium (preferQuantumDefects=True, cpp_numerov=True)
backward compatibility: before only one class for Potassium existed and it corresponded to Potassium 39

class arc.alkali_atom_data.Potassium39 (preferQuantumDefects=True, cpp_numerov=True)

Properties of potassium 39 atoms

a1 = [3.56079437, 3.65670429, 4.12713694, 1.42310446]
model potential parameters from 1

a2 = [1.83909642, 1.67520788, 1.79837462, 1.27861156]
model potential parameters from 1

a3 = [-1.74701102, -2.07416615, -1.69935174, 4.77441476]
model potential parameters from 1

a4 = [-1.03237313, -0.89030421, -0.98913582, -0.94829262]
model potential parameters from 1

abundance = 0.932581
source NIST, Atomic Weights and Isotopic Compositions

alphaC = 5.331
model potential parameters from 1

extraLevels = [[3, 2, 2.5], [3, 2, 1.5]]
levels that are for smaller n than ground level, but are above in energy due to angular part

getAddress (temperature)
Pressure of atomic vapour at given temperature.
Uses equation and values from 3. Values from table 2. (accuracy +- 5%) are used for Na in solid phase. Values from table 3. (accuracy +-1 %) are used for Na in liquid phase.

ionisationEnergy = 4.340663681814173 (eV), weighted average of values in Ref. 11.

mass = 6.470075576376843e-26
source NIST, Atomic Weights and Isotopic Compositions

quantumDefect = [[[2.1801985, 0.13558, 0.0759, 0.117, -0.206, 0.0], [1.713892, 0.233294, 0.16137, 0.5345, -0.234, 0.0], [3.56079437, 3.65670429, 4.12713694, 1.42310446], [1.83909642, 1.67520788, 1.79837462, 1.27861156], [-1.74701102, -2.07416615, -1.69935174, 4.77441476], [-1.03237313, -0.89030421, -0.98913582, -0.94829262]]
quantum defects from Ref. 11.

rc = [0.83167545, 0.85235381, 0.83216907, 6.50294371]
model potential parameters from 1

class arc.alkali_atom_data.Potassium40 (preferQuantumDefects=True, cpp_numerov=True)

Properties of potassium 40 atoms

a1 = [3.56079437, 3.65670429, 4.12713694, 1.42310446]
model potential parameters from 1

a2 = [1.83909642, 1.67520788, 1.79837462, 1.27861156]
model potential parameters from 1
a3 = [-1.74701102, -2.07416615, -1.69935174, 4.77441476]
model potential parameters from

a4 = [-1.03237313, -0.89030421, -0.98913582, -0.94829262]
model potential parameters from

abundance = 0.000117
source NIST, Atomic Weights and Isotopic Compositions

alphaC = 5.331
model potential parameters from

extraLevels = [[3, 2, 2.5], [3, 2, 1.5]]
levels that are for smaller n than ground level, but are above in energy due to angular part

getPressure (temperature)
Pressure of atomic vapour at given temperature.
Uses equation and values from3. Values from table 2. (accuracy +5%) are used for Na in solid phase.
Values from table 3. (accuracy +1%) are used for Na in liquid phase.

ionisationEnergy = 4.340663681814173
(eV), weighted average of values in Ref.11.

mass = 6.63617791491314e-26
source NIST, Atomic Weights and Isotopic Compositions

quantumDefect = [[[2.1801985, 0.13558, 0.0759, 0.117, -0.206, 0.0],
[1.713892, 0.233294, 0.16137, 0.5345, -0.234, 0.0],
[0.010098, -0.100224, 1.56334, -12.6851, 0.0, 0.0],
[0.0, 0.0, 0.0, 0.0, 0.0, 0.0]]
quantum defects from Ref.11.

rc = [0.83167545, 0.85235381, 0.83216907, 6.50294371]
model potential parameters from

scaledRydbergConstant = 13.6055062456062
in eV

class arc.alkali_atom_data.Potassium41 (preferQuantumDefects=True,
cpp_numerov=True)

Properties of potassium 41 atoms

a1 = [3.56079437, 3.65670429, 4.12713694, 1.42310446]
model potential parameters from

a2 = [1.83909642, 1.67520788, 1.79837462, 1.27861156]
model potential parameters from

a3 = [-1.74701102, -2.07416615, -1.69935174, 4.77441476]
model potential parameters from

a4 = [-1.03237313, -0.89030421, -0.98913582, -0.94829262]
model potential parameters from

abundance = 0.067302
source NIST, Atomic Weights and Isotopic Compositions

alphaC = 5.331
model potential parameters from

extraLevels = [[3, 2, 2.5], [3, 2, 1.5]]
levels that are for smaller n than ground level, but are above in energy due to angular part

getPressure (temperature)
Pressure of atomic vapour at given temperature.
Uses equation and values from3. Values from table 2. (accuracy +5%) are used for Na in solid phase.
Values from table 3. (accuracy +1%) are used for Na in liquid phase.

ionisationEnergy = 4.340663681814173
(eV), weighted average of values in Ref.11.
mass = 6.801870999040102e-26
source NIST, Atomic Weights and Isotopic Compositions

quantumDefect = \[
\begin{bmatrix}
2.1801985, 0.13558, 0.0759, 0.117, -0.206, 0.0 \\
1.713892, 0.233294, 0.16137, 0.5345, -0.234, 0.0 \\
1.0053, -19.0244, 0.0 \\
0.010098, -0.100224, 1.56334, -12.6851, 0.0, 0.0 \\
0.0, 0.0, 0.0, 0.0, 0.0, 0.0 \\
\end{bmatrix}
\]
quantum defects from Ref. 11.

rc = [0.83167545, 0.85235381, 0.83216907, 6.50294371]
model potential parameters from 1

scaledRydbergConstant = 13.605510795147651
in eV

class arc.alkali_atom_data.Rubidium(preferQuantumDefects=True, cpp_numerov=True)
backward compatibility: before there was only one Rubidium class, and that one corresponded to Rubidium85

class arc.alkali_atom_data.Rubidium85 (preferQuantumDefects=True, cpp_numerov=True)

Properites of rubidium 85 atoms

a1 = [3.69628474, 4.44088978, 3.78717363, 2.39848933]
model potential parameters from 1

a2 = [1.64915255, 1.92828831, 1.57027864, 1.76810544]
model potential parameters from 1

a3 = [-9.86069196, -16.7959777, -11.6558897, -12.0710678]
model potential parameters from 1

a4 = [0.19579987, -0.8163314, 0.52942835, 0.77256589]
model potential parameters from 1

abundance = 0.7217
source NIST, Atomic Weights and Isotopic Compositions

alphaC = 9.076
model potential parameters from 1

extraLevels = \[[4, 2, 2.5], [4, 2, 1.5], [4, 3, 3.5], [4, 3, 2.5]\]
levels that are for smaller n than ground level, but are above in energy due to angular part

getPressure (temperature)
Pressure of atomic vapour at given temperature.
Uses equation and values from 3. Values from table 2. (accuracy +5%) are used for Rb in solid phase. Values from table 3. (accuracy +1 %) are used for Rb in liquid phase.

ionisationEnergy = 4.177126489738963
(eV) Ref. 15

mass = 1.409993418160543e-25
source NIST, Atomic Weights and Isotopic Compositions

quantumDefect = \[
\begin{bmatrix}
3.1311804, 0.1784, 0.0, 0.0, 0.0, 0.0 \\
2.6548849, 0.29, 0.0, 0.0, 0.0, 0.0 \\
1.34809171, -0.596, 0.0, 0.0, 0.0, 0.0 \\
0.0165437, -0.086, 0.0, 0.0, 0.0, 0.0 \\
0.00405, 0.0, 0.0, 0.0, 0.0, 0.0 \\
\end{bmatrix}
\]
quantum defects for $n_F$ states are from 5. Quantum defects for $n_G$ states are from 7. All other quantum defects are from 4.

rc = [1.66242117, 1.50195124, 4.86851938, 4.79831327]
model potential parameters from 1

scaledRydbergConstant = 13.605605108199638
in eV

class arc.alkali_atom_data.Rubidium87 (preferQuantumDefects=True,
cpp_numerov=True)

Properties of rubidium 87 atoms

a1 = [3.69628474, 4.44088978, 3.78717363, 2.39848933]
model potential parameters from\(^1\)
a2 = [1.64915255, 1.92828831, 1.57027864, 1.76810544]
model potential parameters from\(^1\)
a3 = [-9.86069196, -16.7959777, -11.6558897, -12.0710678]
model potential parameters from\(^1\)
a4 = [0.19579987, -0.8163314, 0.52942835, 0.77256589]
model potential parameters from\(^1\)

abundance = 0.2783
source NIST, Atomic Weights and Isotopic Compositions\(^14\)

alphaC = 9.076
model potential parameters from\(^1\)

extraLevels = [[4, 2, 2.5], [4, 2, 1.5], [4, 3, 3.5], [4, 3, 2.5]]
levels that are for smaller n than ground level, but are above in energy due to angular part

getPressure (temperature)
Pressure of atomic vapour at given temperature.
Uses equation and values from\(^3\). Values from table 2. (accuracy +/- 5%) are used for Rb in solid phase. Values from table 3. (accuracy +/- 1 %) are used for Rb in liquid phase.

ionisationEnergy = 4.177127287605897
(eV) Ref.\(^6\)

mass = 1.4431608720613343e-25
source NIST, Atomic Weights and Isotopic Compositions\(^14\)

quantumDefect = [[3.1311804, 0.1784, 0.0, 0.0, 0.0, 0.0],
[2.6548849, 0.29, 0.0, 0.0, 0.0, 0.0],
[1.34809171, 0.29, -0.596, 0.0, 0.0, 0.0],
[0.0165437, -0.086, 0.0, 0.0, 0.0, 0.0],
[0.00405, 0.0, 0.0, 0.0, 0.0, 0.0]]
quantum defects for \(nF\) states are from\(^5\). Quantum defects for \(nG\) states are from\(^7\). All other quantum defects are from\(^4\)

rc = [1.66242117, 1.50195124, 4.86851938, 4.79831327]
model potential parameters from\(^1\)

scaledRydbergConstant = 13.60560712837914
in eV (M_ion core = m_atomic - m_electron)

class arc.alkali_atom_data.Sodium (preferQuantumDefects=True, cpp_numerov=True)

Properties of sodium 23 atoms

a1 = [4.82223117, 5.08382502, 3.53324124, 1.11056646]
model potential parameters from\(^1\)
a2 = [2.45449865, 2.18226881, 2.48697936, 1.05458759]
model potential parameters from\(^1\)
a3 = [-1.12255048, -1.19534623, -0.75688448, 1.73203428]
model potential parameters from\(^1\)
a4 = [-1.42633139, -1.03142861, -1.27852357, -0.09265696]
model potential parameters from\(^1\)

---


1.3. Detailed documentation of functions
abundance = 1.0
source NIST, Atomic Weights and Isotopic Compositions

alphaC = 0.9448
model potential parameters from

getPressure(temperature)
Pressure of atomic vapour at given temperature.
Uses equation and values from. Values from table 2. (accuracy +/- 5%) are used for Na in solid phase.
Values from table 3. (accuracy +/- 1 %) are used for Na in liquid phase.

ionisationEnergy = 5.139075550664961 (eV) from Ref.\textsuperscript{11}

mass = 3.8175409413353766e-26
source NIST, Atomic Weights and Isotopic Compositions

quantumDefect = \[
\begin{bmatrix}
1.347964, & 0.060673, & 0.0233, & -0.0085, & 0.0, & 0.0 \\
0.85538, & 0.11363, & 0.0384, & 0.1412, & 0.0, & 0.0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0.7958, & -4.0513, & 0.0, & 0.0, & 0.0, & 0.0 \\
0.001453, & 0.017312, & -0.7809, & 7.021, & 0.0, & 0.0 \\
0.0, & 0.0, & 0.0, & 0.0, & 0.0, & 0.0 \\
\end{bmatrix}
\]
Quantum defects are from Ref.\textsuperscript{11}. Note that we are using modified Rydberg-Ritz formula. In literature both modified and non-modified coefficients appear. For more details about the two equations see page 301. of Ref.\textsuperscript{11}.

rc = [0.45489422, 0.45798739, 0.71875312, 28.6735059] model potential parameters from

scaledRydbergConstant = 13.605368351064202 (eV)

1.3.3 Single atom calculations

Overview

StarkMap Methods

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>StarkMap.defineBasis(n, l, m, nMin, ...)</td>
<td>Initializes basis of states around state of interest</td>
</tr>
<tr>
<td>StarkMap.diagonalise(eFieldList, ...)</td>
<td>Finds atom eigenstates in a given electric field</td>
</tr>
<tr>
<td>StarkMap.plotLevelDiagram(units, ...)</td>
<td>Makes a plot of a stark map of energy levels</td>
</tr>
<tr>
<td>StarkMap.showPlot(interactive)</td>
<td>Shows plot made by plotLevelDiagram</td>
</tr>
<tr>
<td>StarkMap.savePlot(filename)</td>
<td>Saves plot made by plotLevelDiagram</td>
</tr>
<tr>
<td>StarkMap.exportData(fileBase, exportFormat)</td>
<td>Exports StarkMap calculation data.</td>
</tr>
<tr>
<td>StarkMap.getPolarizability([maxField, ...])</td>
<td>Returns the polarizability of the state (set during the initialization process)</td>
</tr>
</tbody>
</table>

LevelPlot Methods

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>LevelPlot.makeLevels(nFrom, nTo, lFrom, lTo)</td>
<td>Constructs energy level diagram in a given range</td>
</tr>
<tr>
<td>LevelPlot.drawLevels()</td>
<td>Draws a level diagram plot</td>
</tr>
<tr>
<td>LevelPlot.showPlot()</td>
<td>Shows a level diagram plot</td>
</tr>
</tbody>
</table>

Detailed documentation

This module provides calculations of single-atom properties.

Included calculations are Stark maps, level plot visualisations, lifetimes and radiative decays.

class arc.calculations_atom_single.LevelPlot(atomType)
Single atom level plots and decays

For an example see Rydberg energy levels example snippet.

```python
drawLevels()
Draws a level diagram plot
makeLevels(nFrom, nTo, lFrom, lTo)
Constructs energy level diagram in a given range
Parameters
• nFrom (int) – minimal principal quantum number of the states we are interested in
• nTo (int) – maximal principal quantum number of the states we are interested in
• lFrom (int) – minimal orbital angular momentum of the states we are interested in
• lTo (int) – maximal orbital angular momentum of the states we are interested in
showPlot()
Shows a level diagram plot
class arc.calculations_atom_single.StarkMap(atom)
Calculates Stark maps for single atom in a field
This initializes calculation for the atom of a given type. For details of calculation see Zimmerman1. For a quick working example see Stark map example snippet.

```python
```

Examples

State $28 S_{1/2} |m_J| = 0.5$ polarizability calculation

```python
>>> from arc import *
>>> calc = StarkMap(Caesium())
>>> calc.defineBasis(28, 0, 0.5, 0.5, 23, 32, 20)
>>> calc.diagonalise(np.linspace(00., 6000, 600))
>>> print("%.5f MHz cm^2 / V^2 " % calc.getPolarizability())
0.76705 MHz cm^2 / V^2
```

Stark map calculation

```python
>>> from arc import *
>>> calc = StarkMap(Caesium())
>>> calc.defineBasis(28, 0, 0.5, 0.5, 23, 32, 20)
>>> calc.diagonalise(np.linspace(00., 60000, 600))
>>> calc.plotLevelDiagram()
>>> calc.showPlot()
< matplotlib plot will open containing a Stark map >>
```

Examples

Advanced interfacing of Stark map calculations (StarkMap class) Here we show one easy way to obtain the Stark matrix (from diagonal \( \text{mat1} \) and off-diagonal part \( \text{mat2} \) ) and basis states (stored in \( \text{basisStates} \) ), if this middle-product of the calculation is needed for some code build on top of the existing ARC package.

```python
>>> from arc import *
>>> calc = StarkMap(Caesium())
>>> calc.defineBasis(28, 0, 0.5, 0.5, 23, 32, 20)
>>> # Now we have matrix and basis states, that we can used in our own code
>>> # Let's say we want Stark map at electric field of 0.2 V/m
>>> eField = 0.2 # V/m
>>> # We can easily extract Stark matrix
>>> # as diagonal matrix (state detunings)
>>> # + off-diagonal matrix (propotional to electric field)
>>> matrix = calc.mat1+calc.mat2*eField
>>> # and the basis states as array \([ [n,l,j,mj], \ldots ]\)
>>> basisStates = calc.basisStates
>>> # you can do your own calculation now...
```

References

\texttt{basisStates = None}

List of basis states for calculation in the form \([ [n,l,j,mj], \ldots ]\). Calculated by \texttt{defineBasis}.

\texttt{defineBasis(n, l, j, mj, nMin, nMax, maxL, Bz=0, progressOutput=False, debugOutput=False)}

Initializes basis of states around state of interest

Defines basis of states for further calculation. \( n, l, j, mj \) specify state whose neighbourhood and polarizability we want to explore. Other parameters specify basis of calculations. This method stores basis in \texttt{basisStates}, while corresponding interaction matrix is stored in two parts. First part is diagonal electric-field independent part stored in \texttt{mat1}, while the second part \texttt{mat2} corresponds to off-diagonal elements that are proportional to electric field. Overall interaction matrix for electric field \( e\text{Field} \) can be then obtained as \texttt{fullStarkMatrix = mat1 + mat2 \times e\text{Field}}

Parameters

- \texttt{n (int)} – principal quantum number of the state
- \texttt{l (int)} – angular orbital momentum of the state
- \texttt{j (float)} – total angular momentum of the state
- \texttt{mj (float)} – projection of total angular momentum of the state
- \texttt{nMin (int)} – minimal principal quantum number of the states to be included in the basis for calculation
- \texttt{nMax (int)} – maximal principal quantum number of the states to be included in the basis for calculation
- \texttt{maxL (int)} – maximal value of orbital angular momentum for the states to be included in the basis for calculation
- \texttt{Bz (float)} – optional, magnetic field directed along z-axis in units of Tesla. Calculation will be correct only for weak magnetic fields, where paramagnetic term is much stronger then diamagnetic term. Diamagnetic term is neglected.
- \texttt{progressOutput (bool, optional)} – if True prints the progress of calculation; Set to false by default.
- \texttt{debugOutput (bool, optional)} – if True prints additional information usefull for debugging. Set to false by default.
diagonalise (eFieldList, drivingFromState=[0, 0, 0, 0], progressOutput=False, debugOutput=False)
Finds atom eigenstates in a given electric field

Eigenstates are calculated for a list of given electric fields. To extract polarizability of the original state see getPolarizability method. Results are saved in eFieldList, y and highlight.

Parameters
• eFieldList (array) – array of electric field strength (in V/m) for which we want to know energy eigenstates
• progressOutput (bool, optional) – if True prints the progress of calculation; Set to false by default.
• debugOutput (bool, optional) – if True prints additional information useful for debugging. Set to false by default.

eFieldList = None
Saves electric field (in units of V/m) for which energy levels are calculated

See also:
y, highlight, diagonalise

exportData (fileBase, exportFormat='csv')
Exports StarkMap calculation data.

Only supported format (selected by default) is .csv in a human-readable form with a header that saves details of calculation. Function saves three files: 1) filebase_eField.csv; 2) filebase_energyLevels 3) filebase_highlight

For more details on the format, see header of the saved files.

Parameters
• filebase (string) – filebase for the names of the saved files without format extension. Add as a prefix a directory path if necessary (e.g., saving outside the current working directory)
• exportFormat (string) – optional. Format of the exported file. Currently only .csv is supported but this can be extended in the future.

getPolarizability (maxField=10000000000.0, showPlot=False, debugOutput=False, minStateContribution=0.0)
Returns the polarizability of the state (set during the initialization process)

Parameters
• maxField (float, optional) – maximum field (in V/m) to be used for fitting the polarizability. By default, max field is very large, so it will use eigenvalues calculated in the whole range.
• showPlot (bool, optional) – shows plot of calculated eigenValues of the given state (dots), and the fit (solid line) for extracting polarizability
• debugOutput (bool, optional) – if True prints additional information useful for debugging. Set to false by default.

Returns scalar polarizability in units of MHz cm² / V²

Return type float
highlight = None
highlight[i] is an array of values measuring highlighted feature in the eigenstates at electric field intensity eFieldList[i]. E.g., highlight[i][j] measures highlighted feature of the state with energy y[i][j] at electric field eFieldList[i]. What will be highlighted feature is defined in the call of diagonalise (see that part of documentation for details).
indexOfCoupledState = None
Index of coupled state (initial state passed to defineBasis) in basisStates list of basis states

diagonal elements of Stark-matrix (detuning of states) calculated by defineBasis in the basis basisStates.

diagonal elements of Stark-matrix divided by electric field value. To get off diagonal elements multiply this matrix with electric field value. Full Stark matrix is obtained as fullStarkMatrix = mat1 + mat2 * eField. Calculated by defineBasis in the basis basisStates.

plotLevelDiagram(units=1, highlightState=True, progressOutput=False, debugOutput=False, highlightColour='red', addToExistingPlot=False)
Makes a plot of a stark map of energy levels
To save this plot, see savePlot. To print this plot see showPlot.

Parameters

• units (int, optional) – possible values {1, 2} ; if the value is 1 (default) Stark diagram will be plotted in energy units cm \(^{-1}\); if value is 2, Stark diagram will be plotted as energy /\hbar in units of GHz

• highlightState (bool, optional) – False by default. If True, scatter plot colour map will map in red amount of original state for the given eigenState

• progressOutput (bool, optional) – if True prints the progress of calculation; Set to False by default.

• debugOutput (bool, optional) – if True prints additional information usefull for debugging. Set to False by default.

• addToExistingPlot (bool, optional) – if True adds points to existing old plot. Note that then interactive plotting doesn’t work. False by default.

savePlot (filename='StarkMap.pdf')
Saves plot made by plotLevelDiagram

Parameters filename (str, optional) – file location where the plot should be saved

showPlot (interactive=True)
Shows plot made by plotLevelDiagram

y = None
y[i] is an array of eigenValues corresponding to the energies of the atom states at the electric field eFieldList[i]. For example y[i][j] is energy of the j eigenvalue (energy of the state) measured in cm \(^{-1}\) relative to the ionization threshold.

See also:
eFieldList, highlight, diagonalise

arc.calculations_atom_single.printState(n, l, j)
Prints state spectroscopic label for numeric n, l, s label of the state

Parameters

• n (int) – principal quantum number

• l (int) – orbital angular momentum

• j (float) – total angular momentum

arc.calculations_atom_single.printStateString(n, l, j)
Returns state spectroscopic label for numeric n, l, s label of the state
Parameters

- \( n (\text{int}) \) – principal quantum number
- \( l (\text{int}) \) – orbital angular momentum
- \( j (\text{float}) \) – total angular momentum

Returns: label for the state in standard spectroscopic notation

Return type: string

1.3.4 Pair-state basis calculations

Preliminaries

Relative orientation of the two atoms can be described with polar angle \( \theta \) (range \( 0 - \pi \)) and azimuthal angle \( \phi \) (range \( 0 - 2\pi \)). The \( \hat{z} \) axis is here specified relative to the laser driving. For circularly polarized laser light, this is the direction of laser beam propagation. For linearly polarized light, this is the plane of the electric field polarization, perpendicular to the laser direction.

Internal coupling between the two atoms in \(|n, l, j, m_1\rangle\) and \(|nn, ll, jj, m_2\rangle\) is calculated easily for the two atoms positioned so that \( \theta = 0 \), and for other angles Wigner D matrices are used to change a basis and perform calculation in the basis where couplings are more clearly seen.

Overview

PairStateInteractions Methods

- PairStateInteractions.defineBasis(theta, ...): Finds relevant states in the vicinity of the given pair-state.
- PairStateInteractions.getC6perturbatively(...): Calculates \( C_6 \) from second order perturbation theory.
- PairStateInteractions.getLeRoyRadius(): Returns Le Roy radius for initial pair-state.
- PairStateInteractions.diagonalise(rangeR, ...): Finds eigenstates in atom pair basis.
- PairStateInteractions.plotLevelDiagram(...): Plots pair state level diagram.
- PairStateInteractions.showPlot([interactive]): Shows level diagram printed by PairStateInteractions.plotLevelDiagram.
- PairStateInteractions.exportData(fileBase[, ...]): Exports PairStateInteractions calculation data.
- PairStateInteractions.getC6fromLevelDiagram(): Finds \( C_6 \) coefficient for original pair state.

Continued on next page
### StarkMapResonances Methods

- **StarkMapResonances.findResonances(nMin, ...)**
  - Finds near-resonant dipole-coupled pair-states

- **StarkMapResonances.showPlot([interactive])**
  - Plots initial state Stark map and its dipole-coupled resonances

### Detailed documentation

**Pair-state basis level diagram calculations**

Calculates Rydberg spaghetti of level diagrams, as well as pertubative C6 and similar properties. It also allows calculation of Foster resonances tuned by DC electric fields.

### Example

Calculation of the Rydberg eigenstates in pair-state basis for Rubidium in the vicinity of the \( |60 S_{1/2} m_j = 1/2, 60 S_{1/2} m_j = 1/2 \rangle \) state. Colour highlights coupling strength from state 6 \( P_{1/2} m_j = 1/2 \) with \( \pi (q = 0) \) polarized light. eigenstates:

```python
from arc import 
calc1 = PairStateInteractions(Rubidium(), 60, 0, 0.5, 60, 0, 0.5, 0.5, 0.5) 
calc1.defineBasis(0., 0., 4, 5, 10e9) 
# optionally we can save now results of calculation for future use 
saveCalculation(calc1, "mycalculation.pkl") 
calc1.diagonalise(linspace(1,10.0,30),250,progressOutput = True, 
    drivingFromState=[6,1,0.5,0.5,0]) 
calc1.plotLevelDiagram() 
calc1.ax.set_xlim(1,10) 
calc1.ax.set_ylim(-2,2) 
calc1.showPlot()
```

**Parameters**

- **atom** (AlkaliAtom) – Select the alkali metal for energy level diagram calculation

---

• \(n\) (int) – principal quantum number for the first atom
• \(l\) (int) – orbital angular momentum for the first atom
• \(j\) (float) – total angular momentum for the first atom
• \(nn\) (int) – principal quantum number for the second atom
• \(ll\) (int) – orbital angular momentum for the second atom
• \(jj\) (float) – total angular momentum for the second atom
• \(m1\) (float) – projection of the total angular momentum on z-axis for the first atom
• \(m2\) (float) – projection of the total angular momentum on z-axis for the second atom
• \(\text{interactionsUpTo}\) (int) – Optional. If set to 1, includes only dipole-dipole interactions. If set to 2 includes interactions up to quadrupole-quadrupole. Default value is 1.

References

Examples

Advanced interfacing of pair-state interactions calculations (PairStateInteractions class). This is an advanced example intended for building up extensions to the existing code. If you want to directly access the pair-state interaction matrix, constructed by \texttt{defineBasis}, you can assemble it easily from diagonal part (stored in \texttt{matDiagonal}) and off-diagonal matrices whose spatial dependence is \(R^{-3}, R^{-4}, R^{-5}\) stored in that order in \texttt{matR}. Basis states are stored in \texttt{basisStates} array.

```python
>>> from arc import *
>>> calc = PairStateInteractions(Rubidium(), 60,0,0.5, 60,0,0.5, 0.5,0.5, interactionsUpTo = 1)
>>> # theta=0, phi = 0, range of pqn, range of l, deltaE = 25e9
>>> calc.defineBasis(0 ,0 , 5, 5, 25e9, progressOutput=True)
>>> # now calc stores interaction matrix and relevant basis
>>> # we can access this directly and generate interaction matrix
>>> # at distance rval :
>>> rval = 4 # in mum
>>> matrix = calc.matDiagonal
>>> rX = (rval*1.e-6)**3
>>> for matRX in self.matR:
>>> matrix = matrix + matRX/rX
>>> rX *= (rval*1.e-6)
>>> # matrix variable now holds full interaction matrix for
>>> # interacting atoms at distance rval calculated in
>>> # pair-state basis states can be accessed as
>>> basisStates = calc.basisStates
```

atom = None
atom type

\texttt{basisStates} = None
List of pair-states for calculation. In the form \([n1,l1,j1,mj1,n2,l2,j2,mj2], \ldots\]. Each state is an array \([n1,l1,j1,mj1,n2,l2,j2,mj2]\) corresponding to \(|n1,l1,j1,mj1,n2,l2,j2,mj2\rangle\) state. Calculated by \texttt{defineBasis}.

\texttt{channel} = None
states relevant for calculation, defined in J basis (not resolving \(mj\)). Used as intermediary for full interaction matrix calculation by \texttt{defineBasis}.

\texttt{coupling} = None
List of matrices defining coupling strengths between the states in J basis (not resolving \(mj\)). Basis is given by \texttt{channel}. Used as intermediary for full interaction matrix calculation by \texttt{defineBasis}.
**defineBasis** *(theta, phi, nRange, lrange, energyDelta, Bz=0, progressOutput=False, debugOutput=False)*

Finds relevant states in the vicinity of the given pair-state

Finds relevant pair-state basis and calculates interaction matrix. Pair-state basis is saved in `basisStates`. Interaction matrix is saved in parts depending on the scaling with distance. Diagonal elements `matDiagonal`, corresponding to relative energy defects of the pair-states, don’t change with interatomic separation. Off diagonal elements can depend on distance as $R^{-3}, R^{-4}$ or $R^{-5}$, corresponding to dipole-dipole ($C_3$), dipole-quadrupole ($C_4$) and quadrupole-quadrupole coupling ($C_6$) respectively. These parts of the matrix are stored in `matR` in that order. I.e. `matR[0]` stores dipole-dipole coupling ($\propto R^{-3}$), `matR[0]` stores dipole-quadrupole couplings etc.

**Parameters**

- **theta** (float) – relative orientation of the two atoms (see figure on top of the page), range 0 to $\pi$
- **phi** (float) – relative orientation of the two atoms (see figure on top of the page), range 0 to $2\pi$
- **nRange** (int) – how much below and above the given principal quantum number of the pair state we should be looking?
- **lrange** (int) – what is the maximum angular orbital momentum state that we are including in calculation
- **energyDelta** (float) – what is maximum energy difference ($\Delta E/h$ in Hz) between the original pair state and the other pair states that we are including in calculation
- **Bz** (float) – optional, magnetic field directed along z-axis in units of Tesla. Calculation will be correct only for weak magnetic fields, where paramagnetic term is much stronger than diamagnetic term. Diamagnetic term is neglected.
- **progressOutput** (bool) – optional, False by default. If true, prints information about the progress of the calculation.
- **debugOutput** (bool) – optional, False by default. If true, similar to progressOutput=True, this will print information about the progress of calculations, but with more verbose output.

See also:

alkali_atom_functions.saveCalculation and alkali_atom_functions.loadSavedCalculation for information on saving intermediate results of calculation for later use.

**diagonalise** *(rangeR, noOfEigenvectors, drivingFromState=[0, 0, 0, 0], eigenstateDetuning=0.0, sortEigenvectors=False, progressOutput=False, debugOutput=False)*

Finds eigenstates in atom pair basis.

ARPACK (`scipy.sparse.linalg.eigsh`) calculation of the `noOfEigenvectors` eigenvectors closest to the original state. If `drivingFromState` is specified as $[n, l, j, mj]$ coupling between the pair-states and the situation where one of the atoms in the pair state basis is in $|n, l, j, mj\rangle$ state due to driving with a laser field that drives $q$ transition ($+1, 0, -1$ for $\sigma^+$, $\pi$ and $\sigma^-$ transitions respectively) is calculated and marked by the colourmaping these values on the obtained eigenvectors.

**Parameters**

- **rangeR** (array) – Array of values for distance between the atoms (in $\mu m$) for which we want to calculate eigenstates.
- **noOfEigenvectors** (int) – number of eigen vectors closest to the energy of the original (unperturbed) pair state. Has to be smaller then the total number of states.
eigenstateDetuning (float, optional) – Default is 0. This specifies detuning from the initial pair-state (in Hz) around which we want to find noOfEigenvectors eigenvectors. This is useful when looking only for couple of off-resonant features.

drivingFromState ([int, int, float, float, int]) – Optional. State of the one of the atoms from the original pair-state basis from which we try to drive to the excited pair-basis manifold. By default, program will calculate just contribution of the original pair-state in the eigenstates obtained by diagonalization, and will highlight it’s admixture by colour mapping the obtained eigenstates plot.

sortEigenvectors (bool) – optional, False by default. Tries to sort eigenvectors so that given eigen vector index corresponds to adiabatically changing eigenstate, as determined by maximising overlap between old and new eigenvectors.

progressOutput (bool) – optional, False by default. If true, prints information about the progress of the calculation.

debugOutput (bool) – optional, False by default. If true, similar to progressOutput=True, this will print information about the progress of calculations, but with more verbose output.

exportData (fileBase, exportFormat='csv')
Exports PairStateInteractions calculation data.

getC3fromLevelDiagram (rStart, rStop, showPlot=False, minStateContribution=0.0, resonantBranch=1)
Finds $C_3$ coefficient for original pair state.

Parameters

- filebase (string) – filebase for the names of the saved files without format extension. Add as a prefix a directory path if necessary (e.g. saving outside the current working directory)
- exportFormat (string) – optional. Format of the exported file. Currently only .csv is supported but this can be extended in the future.
- rStart (float) – smallest inter-atomic distance to be used for fitting
- rStop (float) – maximum inter-atomic distance to be used for fitting
- showPlot (bool) – If set to true, it will print the plot showing fitted energy level and the obtained best fit. Default is False
- minStateContribution (float) – valid values are in the range [0,1). It specifies minimum amount of the original state in the given energy state necessary for the state to be considered for the adiabatic continuation of the original unperturbed pair state.
• **resonantBranch**(int) – optional, default +1. For resonant interactions we have two branches with identical state contributions. In this case, we will select only positively detuned branch (for resonantBranch = +1) or negatively detuned branch (for resonantBranch = -1) depending on the value of resonantBranch optional parameter.

**Returns** $C_3$ measured in GHz $\mu$m$^6$ on success; If unsuccessful returns False.

**Return type** float

---

**get$C_6$fromLevelDiagram**(rStart, rStop, showPlot=False, minStateContribution=0.0)

Finds $C_6$ coefficient for original pair state.

Function first finds for each distance in the range $[rStart, rStop]$ the eigen state with highest contribution of the original state. One can set optional parameter minStateContribution to value in the range $[0,1)$, so that function finds only states if they have contribution of the original state that is bigger then minStateContribution.

Once original pair-state is found in the range of interatomic distances, from smallest rStart to the biggest rStop, function will try to perform fitting of the corresponding state energy $E(R)$ at distance $R$ to the function $A + C_6/R^6$ where $A$ is some offset.

**Parameters**

- **rStart**(float) – smallest inter-atomic distance to be used for fitting
- **rStop**(float) – maximum inter-atomic distance to be used for fitting
- **showPlot**(bool) – If set to true, it will print the plot showing fitted energy level and the obtained best fit. Default is False
- **minStateContribution**(float) – valid values are in the range $[0,1)$. It specifies minimum amount of the original state in the given energy state necessary for the state to be considered for the adiabatic continuation of the original unperturbed pair state.

**Returns** $C_6$ measured in GHz $\mu$m$^6$ on success; If unsuccessful returns False.

**Return type** float

---

**get$C_6$perturbatively**(theta, phi, nRange, energyDelta)

Calculates $C_6$ from second order perturbation theory.

Calculates $C_6 = \sum_{r',r''} |\langle r',r''|V|r1,r2\rangle|^2/\Delta_{r',r''}$, where $\Delta_{r',r''} \equiv E(r',r'') - E(r1,r2)$

This calculation is faster then full diagonalization, but it is valid only far from the so called spaghetti region that occurs when atoms are close to each other. In that region multiple levels are strongly coupled, and one needs to use full diagonalization. In region where perturbative calculation is correct, energy level shift can be obtained as $V(R) = -C_6/R^6$

See perturbative $C_6$ calculations example snippet.

**Parameters**

- **theta**(float) – orientation of inter-atomic axis with respect to quantization axis (z) in Euler coordinates (measured in units of radian)
• \textbf{phi} (\textit{float}) – orientation of inter-atomic axis with respect to quantization axis (\( z \)) in Euler coordinates (measured in units of radian)

• \textbf{nRange} (\textit{int}) – how much below and above the given principal quantum number of the pair state we should be looking

• \textbf{energyDelta} (\textit{float}) – what is maximum energy difference (\( \Delta E/\hbar \) in Hz) between the original pair state and the other pair states that we are including in calculation

\textbf{Returns} \( C_6 \) measured in \( \text{GHz} \ \mu \text{m}^6 \)

\textbf{Return type} \textit{float}

\textbf{Example}

If we want to quickly calculate \( C_6 \) for two Rubidium atoms in state \( 62D_{3/2}m_j = 3/2 \), positioned in space along the shared quantization axis:

```python
from arc import *
calculaton = PairStateInteractions(Rubidium(), 62, 2, 1.5, 62, 2, 1.5, 1.
\rightarrow 5, 1.5)
c6 = calculation.getC6perturbatively(0,0, 5, 25e9)
print "C_6 = %.0f GHz (\mu m)^6" % c6
```

Which returns:

\( C_6 = 767 \text{ GHz} \ \mu \text{m}^6 \)

Quick calculation of angular anisotropy of for Rubidium \( D_{2/5}, m_j = 5/2 \) states:

```python
# Rb 60 D_{2/5}, mj=2.5 , 60 D_{2/5}, mj=2.5 pair state
calculaton1 = PairStateInteractions(Rubidium(), 60, 2, 2.5, 60, 2, 2.5, 2.
\rightarrow 5, 2.5)
# list of atom orientations
thetalist = np.linspace(0,pi,30)
# do calculation of C6 pertubatively for all atom orientations
c6 = []
for theta in thetalist:
    value = calculaton1.getC6perturbatively(theta,0,5,25e9)
    c6.append(value)
print("theta = %.2f\pi C6 = %.2f GHz \mu m^6" % (theta/\pi,
\rightarrow value))
# plot results
plot(thetalist/\pi,c6,"b-")
title("Rb, pairstate 60 D(5/2),m_j = 5/2, 60 D(5/2),m_j = 5/2")
xlabel("\Theta /\pi")
ylabel("$C_6$ (GHz $\mu$m$^6$)
show()
```

\textbf{getLeRoyRadius}()

Returns Le Roy radius for initial pair-state.

Le Roy radius\(^2\) is defined as \( 2\left(\langle r_1^2 \rangle^{1/2} + \langle r_2^2 \rangle^{1/2} \right) \), where \( r_1 \) and \( r_2 \) are electron coordinates for the first and the second atom in the initial pair-state. Below this radius, calculations are not valid since electron wavefunctions start to overlap.

\textbf{Returns} \textit{LeRoy radius measured in \( \mu \text{m} \)}

\textbf{Return type} \textit{float}

getVdwFromLevelDiagram\((r\text{Start}, r\text{Stop}, show\text{Plot}=False, min\text{State}\text{Contribution}=0.0)\)

Finds \(r_{vdW}\) coefficient for original pair state.

Function first finds for each distance in the range \([r\text{Start}, r\text{Stop}]\) the eigen state with highest contribution of the original state. One can set optional parameter \(min\text{State}\text{Contribution}\) to value in the range \([0,1)\), so that function finds only states if they have contribution of the original state that is bigger than \(min\text{State}\text{Contribution}\).

Once original pair state is found in the range of interatomic distances, from smallest \(r\text{Start}\) to the biggest \(r\text{Stop}\), function will try to perform fitting of the corresponding state energy \(E(R)\) at distance \(R\) to the function

\[
A + B \frac{1 - \sqrt{1 + (r_{vdW}/R)^6}}{1 - \sqrt{1 + r_{vdW}^6}}
\]

where \(A\) and \(B\) are some offset.

**Parameters**

- \(r\text{Start}\) (float) – smallest inter-atomic distance to be used for fitting
- \(r\text{Stop}\) (float) – maximum inter-atomic distance to be used for fitting
- \(show\text{Plot}\) (bool) – If set to true, it will print the plot showing fitted energy level and the obtained best fit. Default is False
- \(min\text{State}\text{Contribution}\) (float) – valid values are in the range \([0,1)\). It specifies minimum amount of the original state in the given energy state necessary for the state to be considered for the adiabatic continuation of the original unperturbed pair state.

**Returns** \(r_{vdW}\) measured in \(\mu m\) on success; If unsuccessful returns False.

**Return type** float

**Note:** In order to use this functions, highlighting in \textit{diagonalise} should be based on the original pair state contribution of the eigenvectors (that this, \textit{drivingFromState} parameter should not be set, which corresponds to \textit{drivingFromState} = \([0,0,0,0]\)).

**interactionsUpTo = None**

" Specifies up to which approximation we include in pair-state interactions. By default value is 1, corresponding to pair-state interactions up to dipole-dipole coupling. Value of 2 is also supported, corresponding to pair-state interactions up to quadrupole-quadrupole coupling.

\(j = None\)

total angular momentum of the first atom

**Type** pair-state definition

\(jj = None\)

total angular momentum of the second atom

**Type** pair-state definition

\(l = None\)

orbital angular momentum of the first atom

**Type** pair-state definition

\(ll = None\)

orbital angular momentum of the second atom

**Type** pair-state definition

\(m1 = None\)

projection of the total ang. momentum for the \textit{first} atom
m2 = None
projection of the total angular momentum for the second atom

matDiagonal = None
Part of interaction matrix in pair-state basis that doesn’t depend on inter-atomic distance. E.g. diagonal elements of the interaction matrix, that describe energies of the pair states in unperturbed basis, will be stored here. Basis states are stored in `basisStates`. Calculated by `defineBasis`.

matR = None
Stores interaction matrices in pair-state basis that scale as $1/R^3$, $1/R^4$ and $1/R^5$ with distance in `matR[0]`, `matR[1]` and `matR[2]` respectively. These matrices correspond to dipole-dipole ($C_3$), dipole-quadrupole ($C_4$) and quadrupole-quadrupole ($C_5$) interactions coefficients. Basis states are stored in `basisStates`. Calculated by `defineBasis`.

matrixElement = None
`matrixElement[i]` gives index of state in channel basis (that doesn’t resolve $m_j$ states), for the given index $i$ of the state in `basisStates` ($m_j$ resolving) basis.

n = None
principal quantum number of the first atom

nn = None
principal quantum number of the second atom

originalPairStateIndex = None
index of the original n,l,j,m1,nn,ll,jj,m2 pair-state in the `basisStates` basis.

plotLevelDiagram (highlightColor='red', highlightScale='linear')
Plots pair state level diagram
Call `showPlot` if you want to display a plot afterwards.

Parameters

- **highlightColor**(string) – optional, specifies the colour used for state highlighting
- **highlightScale**(string) – optional, specifies scaling of state highlighting. Default is ‘linear’. Use ‘log-2’ or ‘log-3’ for logarithmic scale going down to 1e-2 and 1e-3 respectively. Logarithmic scale is useful for spotting weakly admixed states.

savePlot (filename='PairStateInteractions.pdf')
Saves plot made by `plotLevelDiagram`

Parameters **filename**(str, optional) – file location where the plot should be saved

showPlot (interactive=True)
Shows level diagram printed by `PairStateInteractions.plotLevelDiagram`
By default, it will output interactive plot, which means that clicking on the state will show the composition of the clicked state in original basis (dominant elements)

Parameters **interactive**(bool) – optional, by default it is True. If true, plotted graph will be interactive, i.e. users can click on the state to identify the state composition

Note: interactive=True has effect if the graphs are explored in usual matplotlib pop-up windows. It doesn’t have effect on inline plots in Jupyter (IPython) notebooks.
class arc.calculations_atom_pairstate.StarkMapResonances(atom1, state1, atom2, state2)

Calculates pair state Stark maps for finding resonances

Tool for finding conditions for Foster resonances. For a given pair state, in a given range of the electric fields, looks for the pair-state that are close in energy and coupled via dipole-dipole interactions to the original pair-state.

See Stark resonances example snippet.

Parameters


  the first atom in the pair-state

* state1 ([int, int, float, float]) – specification of the state of the first state as an array of values \([n, l, j, m_j]\)


  the second atom in the pair-state

* state2 ([int, int, float, float]) – specification of the state of the first state as an array of values \([n, l, j, m_j]\)

Note: In checking if certain state is dipole coupled to the original state, only the highest contributing state is checked for dipole coupling. This should be fine if one is interested in resonances in weak fields. For stronger fields, one might want to include effect of coupling to other contributing base states.

findResonances (nMin, nMax, maxL, eFieldList, energyRange=[-5000000000.0, 5000000000.0], Bz=0, progressOutput=False)

Finds near-resonant dipole-coupled pair-states

For states in range of principal quantum numbers \([nMin, nMax']\) and orbital angular momentum \([0, 'maxL']\), for a range of electric fields given by eFieldList function will find near-resonant pair states.

Only states that are in the range given by energyRange will be extracted from the pair-state Stark maps.

Parameters

* nMin (int) – minimal principal quantum number of the state to be included in the StarkMap calculation

* nMax (int) – maximal principal quantum number of the state to be included in the StarkMap calculation

* maxL (int) – maximum value of orbital angular momentum for the states to be included in the calculation

* eFieldList ([float]) – list of the electric fields (in V/m) for which to calculate level diagram (StarkMap)

* Bz (float) – optional, magnetic field directed along z-axis in units of Tesla. Calculation will be correct only for weak magnetic fields, where paramagnetic term is much stronger than diamagnetic term. Diamagnetic term is neglected.
• `energyRange ((float, float))` - optional argument. Minimal and maximal energy of that some dipole-coupled state should have in order to keep it in the plot (in units of Hz). By default it finds states that are ±5 GHz.

• `progressOutput (bool, optional)` - if True prints the progress of calculation; Set to false by default.

`showPlot (interactive=True)`

Plots initial state Stark map and its dipole-coupled resonances

**Parameters**

- `interactive (optional, bool)` - if True (by default) points on plot will be clickable so that one can find the state labels and their composition (if they are heavily admixed).

### 1.4 How to contribute to the project

Ideally, this package/library will grow into a community project, as a community-maintained resource for atomic physics community. Full code will be accessible from GitHub, so please fork the project, and submit improvements, additional modules, new features, or just suggest ideas. We have a list of features that can be potentially included.

#### 1.4.1 Ideas for development

This is incomplete list of some of the modules that can be added to the library:

- Dressing potentials
- Magic wavelengths
- Atom-wall interactions
- Photoionization
- Collisional cross-sections
- Tensor polarisability
- ... (add your own ideas)

#### 1.4.2 Naming conventions

For the sake of consistency, readability and cross-linking with the written literature, please follow the following for contributions:

- Names and method/subdivision should reflect *structure of knowledge in atomic physics*, NOT low-level implementation structure.

- Names should be sensible to atomic physicists (even if they are not familiar with coding).

- Use long self-descriptive variable names (so that the code is self-documented and readable in itself) and write short comment on functions of code subsections.

- Use Google style docstrings for code documentation (we are using Sphinx Napoleon extension for generating documentation)

- Add references to original papers in comments and docstrings.

Finally, this is the naming convention of the original package. For consistency, we suggest following the same naming convention.

- Submodules are lower case, separated by underscore. Example:
import my_module_name

• Classes are named in CamelCase, for example:

```python
class MyNewClass:
    ...
```

• Class methods that return a value start with get in their name, and follow camelCase convention, for example:

```python
def getSumOfTwoNumbers(a, b):
    return a + b
```

• Class methods don’t return a value are named in camelCase, for example:

```python
def defineBasis():
    ...
```
Fig. 1: Overview of modules and interdependencies in the \texttt{arc} package. Click on image to enlarge.
CHAPTER 3

Indices and tables

- genindex
- modindex
- search
Credits

Authors  Nikola Šibalić, Jonathan D. Pritchard, Charles S. Adams, Kevin J. Weatherill
Licence  BSD 3-Clause
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Python Module Index

a
arc.alkali_atom_data, 21
arc.alkali_atom_functions, 7
arc.calculations_atom_pairstate, 34
arc.calculations_atom_single, 28
Index
Alkali Rydberg Calculator (ARC) Documentation, Release 2.0.6

basisStates (arc.calculations_atom_single.StarkMap attribute), 30

C
Caesium (class in arc.alkali_atom_data), 21
channel (arc.calculations_atom_pairstate.PairStateInteractions attribute), 35
corePotential() (arc.alkali_atom_functions.AlkaliAtom method), 7
coupling (arc.calculations_atom_pairstate.PairStateInteractions attribute), 35
cpp_numerov (arc.alkali_atom_functions.AlkaliAtom attribute), 8
defineBasis() (arc.calculations_atom_pairstate.PairStateInteractions method), 35
defineBasis() (arc.calculations_atom_single.StarkMap method), 30
diagonalise() (arc.calculations_atom_pairstate.PairStateInteractions method), 36
diagonalise() (arc.calculations_atom_single.StarkMap method), 30
dipoleMatrixElementFile (arc.alkali_atom_functions.AlkaliAtom attribute), 8
drawLevels() (arc.calculations_atom_single.LevelPlot method), 29

effectiveCharge() (arc.alkali_atom_functions.AlkaliAtom method), 8
eFieldList (arc.calculations_atom_single.StarkMap attribute), 31
elementName (arc.alkali_atom_functions.AlkaliAtom attribute), 8
exportData() (arc.calculations_atom_pairstate.PairStateInteractions method), 37
exportData() (arc.calculations_atom_single.StarkMap method), 31
extraLevels (arc.alkali_atom_data.Caesium attribute), 22
extraLevels (arc.alkali_atom_data.Potassium39 attribute), 24
extraLevels (arc.alkali_atom_data.Potassium40 attribute), 25
extraLevels (arc.alkali_atom_data.Potassium41 attribute), 25
extraLevels (arc.alkali_atom_data.Rubidium85 attribute), 26
extraLevels (arc.alkali_atom_data.Rubidium87 attribute), 27
extraLevels (arc.alkali_atom_functions.AlkaliAtom attribute), 8

F
findResonances() (arc.calculations_atom_pairstate.StarkMapResonances method), 42
generateDiagDiag() (arc.calculations_atom_pairstate.StarkMapResonances method), 42
generateDiagDiag() (arc.calculations_atom_single.StarkMap method), 31
generateMatrix() (arc.getMatrix method), 9
getAverageInteratomicSpacing() (arc.alkali_atom_functions.AlkaliAtom method), 8
getAddress() (arc.getAtom method), 5
getAverageSpeed() (arc.alkali_atom_functions.AlkaliAtom method), 8
getC3fromLevelDiagram() (arc.calculations_atom_pairstate.PairStateInteractions method), 37
getc3perturbatively() (arc.calculations_atom_pairstate.PairStateInteractions method), 38
getc6term() (arc.alkali_atom_functions.AlkaliAtom method), 9
dipoleMatrixElement () (arc.alkali_atom_functions.AlkaliAtom method), 10
generateDME() (arc.alkali_atom_functions.AlkaliAtom method), 11
generateDME2() (arc.alkali_atom_functions.AlkaliAtom method), 11
generateDME3() (arc.alkali_atom_functions.AlkaliAtom method), 12
generateDME4() (arc.alkali_atom_functions.AlkaliAtom method), 12
getLiteratureDME() (arc.alkali_atom_functions.AlkaliAtom method), 11
defineBasis() (arc.calculations_atom_pairstate.PairStateInteractions method), 35
defineBasis() (arc.calculations_atom_single.StarkMap method), 30
diagonalise() (arc.calculations_atom_pairstate.PairStateInteractions method), 36
diagonalise() (arc.calculations_atom_single.StarkMap method), 30

drawLevels() (arc.calculations_atom_single.LevelPlot method), 29

effectiveCharge() (arc.alkali_atom_functions.AlkaliAtom method), 8
eFieldList (arc.calculations_atom_single.StarkMap attribute), 31
elementName (arc.alkali_atom_functions.AlkaliAtom attribute), 8
exportData() (arc.calculations_atom_pairstate.PairStateInteractions method), 37
exportData() (arc.calculations_atom_single.StarkMap method), 31
extraLevels (arc.alkali_atom_data.Caesium attribute), 22
extraLevels (arc.alkali_atom_data.Potassium39 attribute), 24
extraLevels (arc.alkali_atom_data.Potassium40 attribute), 25
extraLevels (arc.alkali_atom_data.Potassium41 attribute), 25
extraLevels (arc.alkali_atom_data.Rubidium85 attribute), 26
extraLevels (arc.alkali_atom_data.Rubidium87 attribute), 27
extraLevels (arc.alkali_atom_functions.AlkaliAtom attribute), 8

G
getAverageInteratomicSpacing() (arc.alkali_atom_functions.AlkaliAtom method), 8
getAddress() (arc.getAtom method), 5
generated() (arc.alkali_atom_functions.AlkaliAtom method), 10
generateDME() (arc.alkali_atom_functions.AlkaliAtom method), 11
generateDME2() (arc.alkali_atom_functions.AlkaliAtom method), 11
generateDME3() (arc.alkali_atom_functions.AlkaliAtom method), 12
generateDME4() (arc.alkali_atom_functions.AlkaliAtom method), 12
getLiteratureDME() (arc.alkali_atom_functions.AlkaliAtom method), 11
defineBasis() (arc.calculations_atom_pairstate.PairStateInteractions method), 35
defineBasis() (arc.calculations_atom_single.StarkMap method), 30
diagonalise() (arc.calculations_atom_pairstate.PairStateInteractions method), 36
diagonalise() (arc.calculations_atom_single.StarkMap method), 30

drawLevels() (arc.calculations_atom_single.LevelPlot method), 29

effectiveCharge() (arc.alkali_atom_functions.AlkaliAtom method), 8
eFieldList (arc.calculations_atom_single.StarkMap attribute), 31
elementName (arc.alkali_atom_functions.AlkaliAtom attribute), 8
exportData() (arc.calculations_atom_pairstate.PairStateInteractions method), 37
exportData() (arc.calculations_atom_single.StarkMap method), 31
extraLevels (arc.alkali_atom_data.Caesium attribute), 22
extraLevels (arc.alkali_atom_data.Potassium39 attribute), 24
extraLevels (arc.alkali_atom_data.Potassium40 attribute), 25
extraLevels (arc.alkali_atom_data.Potassium41 attribute), 25
extraLevels (arc.alkali_atom_data.Rubidium85 attribute), 26
extraLevels (arc.alkali_atom_data.Rubidium87 attribute), 27
extraLevels (arc.alkali_atom_functions.AlkaliAtom attribute), 8

Index
getPressure() (arc.alkali_atom_data.Rubidium85 method), 26
getPressure() (arc.alkali_atom_data.Rubidium87 method), 27
getPressure() (arc.alkali_atom_data.Sodium method), 28
getQuadrupoleMatrixElement() (arc.alkali_atom_functions.AlkaliAtom method), 13
getQuantumDefect() (arc.alkali_atom_functions.AlkaliAtom method), 13
getRabiFrequency() (arc.alkali_atom_functions.AlkaliAtom method), 13
getRabiFrequency2() (arc.alkali_atom_functions.AlkaliAtom method), 13
getRadialCoupling() (arc.alkali_atom_functions.AlkaliAtom method), 14
getRadialMatrixElement() (arc.alkali_atom_functions.AlkaliAtom method), 14
getReducedMatrixElementJ() (arc.alkali_atom_functions.AlkaliAtom method), 14
getReducedMatrixElementJ_asymmetric() (arc.alkali_atom_functions.AlkaliAtom method), 14
getReducedMatrixElementL() (arc.alkali_atom_functions.AlkaliAtom method), 15
getStateLifetime() (arc.alkali_atom_functions.AlkaliAtom method), 15
getTransitionFrequency() (arc.alkali_atom_functions.AlkaliAtom method), 16
getTransitionRate() (arc.alkali_atom_functions.AlkaliAtom method), 16
getTransitionWavelength() (arc.alkali_atom_functions.AlkaliAtom method), 17
defVdwFromLevelDiagram() (arc.calculations_atom_pairstate.PairStateInteractions method), 40
getZeemanEnergyShift() (arc.alkali_atom_functions.AlkaliAtom method), 17
groundStateN (arc.alkali_atom_functions.AlkaliAtom attribute), 17

Hydrogen (class in arc.alkali_atom_data), 22

indexOfCoupledState
(arc.calculations_atom_single.StarkMap attribute), 32
interactionsUpTo
(arc.calculations_atom_pairstate.PairStateInteractions attribute), 40
ionisationEnergy
(arc.alkali_atom_data.Caesium attribute), 22
ionisationEnergy
(arc.alkali_atom_data.Hydrogen attribute), 22
ionisationEnergy
(arc.alkali_atom_data.Lithium7 attribute), 23
ionisationEnergy
(arc.alkali_atom_data.Potassium39 attribute), 24
ionisationEnergy
(arc.alkali_atom_data.Potassium40 attribute), 25
ionisationEnergy
(arc.alkali_atom_data.Potassium41 attribute), 25
ionisationEnergy
(arc.alkali_atom_data.Rubidium85 attribute), 26
ionisationEnergy
(arc.alkali_atom_data.Rubidium87 attribute), 27
ionisationEnergy
(arc.alkali_atom_data.Sodium attribute), 28

J

j (arc.calculations_atom_pairstate.PairStateInteractions attribute), 40
jj (arc.calculations_atom_pairstate.PairStateInteractions attribute), 40

L

l (arc.calculations_atom_pairstate.PairStateInteractions attribute), 40
levelDataFromNIST
(arc.alkali_atom_functions.AlkaliAtom attribute), 17
LevelPlot (class in arc.calculations_atom_single), 28
literatureDMEfilename
(arc.alkali_atom_functions.AlkaliAtom attribute), 17
Lithium6 (class in arc.alkali_atom_data), 22
Lithium7 (class in arc.alkali_atom_data), 23
ll (arc.calculations_atom_pairstate.PairStateInteractions attribute), 40

H

highlight (arc.calculations_atom_single.StarkMap attribute), 31
loadSavedCalculation() (in module arc.alkali_atom_functions), 19

M
m1 (arc.calculations_atom_pairstate.PairStateInteractions
attribute), 40
m2 (arc.calculations_atom_pairstate.PairStateInteractions
attribute), 41
makeLevels() (arc.calculations_atom_single.LevelPlot
method), 29
mass (arc.alkali_atom_data.Hydrogen attribute), 22
mass (arc.alkali_atom_data.Lithium6 attribute), 23
mass (arc.alkali_atom_data.Lithium7 attribute), 24
mass (arc.alkali_atom_data.Potassium39 attribute), 24
mass (arc.alkali_atom_data.Potassium40 attribute), 25
mass (arc.alkali_atom_data.Potassium41 attribute), 25
mass (arc.alkali_atom_data.Rubidium85 attribute), 26
mass (arc.alkali_atom_data.Rubidium87 attribute), 27
mass (arc.alkali_atom_data.Sodium attribute), 28
mass (arc.alkali_atom_functions.AlkaliAtom attribute), 17
mat1 (arc.calculations_atom_single.StarkMap
attribute), 32
mat2 (arc.calculations_atom_single.StarkMap
attribute), 32
matDiagonal (arc.calculations_atom_pairstate.PairStateInteractions
attribute), 41
matR (arc.calculations_atom_pairstate.PairStateInteractions
attribute), 41
matrixElement (arc.calculations_atom_pairstate.PairStateInteractions
attribute), 41
minQuantumDefectN (arc.alkali_atom_functions.AlkaliAtom
attribute), 17

N
n (arc.calculations_atom_pairstate.PairStateInteractions
attribute), 41
nn (arc.calculations_atom_pairstate.PairStateInteractions
attribute), 41
NumerovBack() (in module arc.alkali_atom_functions), 18

O
originalPairStateIndex (arc.calculations_atom_pairstate.PairStateInteractions
attribute), 41

P
PairStateInteractions (class in arc.calculations_atom_pairstate), 34
plotLevelDiagram() (arc.calculations_atom_pairstate.PairStateInteractions
method), 41

Q
quadrupoleMatrixElementFile (arc.alkali_atom_functions.AlkaliAtom
attribute), 17
quantumDefect (arc.alkali_atom_data.Caesium
attribute), 22
quantumDefect (arc.alkali_atom_data.Lithium6
attribute), 23
quantumDefect (arc.alkali_atom_data.Lithium7
attribute), 24
quantumDefect (arc.alkali_atom_data.Potassium39
attribute), 24
quantumDefect (arc.alkali_atom_data.Potassium40
attribute), 25
quantumDefect (arc.alkali_atom_data.Potassium41
attribute), 25
quantumDefect (arc.alkali_atom_data.Rubidium85
attribute), 26
quantumDefect (arc.alkali_atom_data.Rubidium87
attribute), 27
quantumDefect (arc.alkali_atom_data.Sodium
attribute), 28
quantumDefect (arc.alkali_atom_functions.AlkaliAtom
attribute), 18

R
radialWavefunction() (arc.alkali_atom_functions.AlkaliAtom
method), 18
rc (arc.alkali_atom_data.Caesium attribute), 22
rc (arc.alkali_atom_data.Lithium6 attribute), 23
rc (arc.alkali_atom_data.Lithium7 attribute), 24
rc (arc.alkali_atom_data.Potassium39 attribute), 24
rc (arc.alkali_atom_data.Potassium40 attribute), 25
rc (arc.alkali_atom_data.Potassium41 attribute), 26
rc (arc.alkali_atom_data.Rubidium85 attribute), 26
rc (arc.alkali_atom_data.Rubidium87 attribute), 27
rc (arc.alkali_atom_data.Sodium attribute), 28
rc (arc.alkali_atom_functions.AlkaliAtom attribute), 18
Rubidium (class in arc.alkali_atom_data), 26
Rubidium85 (class in arc.alkali_atom_data), 26
Rubidium87 (class in arc.alkali_atom_data), 27

S
saveCalculation() (in module arc.alkali_atom_functions), 20
savePlot() (arc.calculations_atom_pairstate.PairStateInteractions method), 41
savePlot() (arc.calculations_atom_single.StarkMap method), 32
scaledRydbergConstant
(arc.alkali_atom_data.Caesium attribute), 22
scaledRydbergConstant
(arc.alkali_atom_data.Potassium40 attribute), 25
scaledRydbergConstant
(arc.alkali_atom_data.Potassium41 attribute), 26
scaledRydbergConstant
(arc.alkali_atom_data.Rubidium85 attribute), 26
scaledRydbergConstant
(arc.alkali_atom_data.Rubidium87 attribute), 27
scaledRydbergConstant
(arc.alkali_atom_data.Sodium attribute), 28
scaledRydbergConstant
(arc.alkali_atom_functions.AlkaliAtom attribute), 18
setup_data_folder() (in module arc.alkali_atom_functions), 20
showPlot() (arc.calculations_atom_pairstate.PairStateInteractions method), 41
showPlot() (arc.calculations_atom_pairstate.StarkMapResonances method), 43
showPlot() (arc.calculations_atom_single.LevelPlot method), 29
showPlot() (arc.calculations_atom_single.StarkMap method), 32
Sodium (class in arc.alkali_atom_data), 27
StarkMap (class in arc.calculations_atom_single), 29
StarkMapResonances (class in arc.calculations_atom_pairstate), 41

U
updateDipoleMatrixElementsFile()
(arc.alkali_atom_functions.AlkaliAtom method), 18

Y
y (arc.calculations_atom_single.StarkMap attribute), 32