My Project

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1.1 Namespace List

Here is a list of all documented namespaces with brief descriptions:

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2.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 3

Namespace Documentation

3.1 atom_2e Module Reference

This program calculates bound (b), single-ionization (si) and double-ionization (di) probabilities based on the tdse.nc output of the tdse calculation of a 2e-system.

Data Types

- type symmetry_ls2e

Functions/Subroutines

- subroutine **init_symmetry_ls2e** (this, l_2e, s_2e, n_e2e, n_c2e)
- subroutine **init_w2e_configurations** (this, li)

3.1.1 Detailed Description

This program calculates bound (b), single-ionization (si) and double-ionization (di) probabilities based on the tdse.nc output of the tdse calculation of a 2e-system.

$P_{di} = \sum_{E>0,nl>0} |\langle\phi_0|\psi(t)\rangle|^2$

Chapter 4

Class Documentation

4.1 atom_2e::symmetry_ls2e Type Reference

Public Attributes

- integer **l**
- integer **s**
- integer **net**
- real(dpk), dimension(:), allocatable **ent**
- complex(dpk), dimension(:), allocatable **ct**
- real(dpk), dimension(:), allocatable **pt**
- integer **nev**
- integer **ncf**
- integer **nch**
- integer, dimension(:), allocatable **n1**
- integer, dimension(:), allocatable **l1**
- integer, dimension(:), allocatable **n2**
- integer, dimension(:), allocatable **l2**
- real(dpk), dimension(:), allocatable **ev**
- real(dpk), dimension(:,:), allocatable **cv**
- real(dpk), dimension(:), allocatable **pvt**
- real(dpk), dimension(:), allocatable **var**
- real(dpk), dimension(:), allocatable **f**
- real(dpk), dimension(ic), allocatable **p** = \sum_{ie} | cv(ie, ic) * ct(ie) |^2 \f$
- real(dpk), dimension(:), allocatable **pvt_b**
- real(dpk), dimension(:), allocatable **pvt_s**
- real(dpk), dimension(:), allocatable **pvt_d**
- real(dpk), dimension(:), allocatable **pop_c2e**

The documentation for this type was generated from the following file:

- tdse_pop_sdi.f90

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