User manual

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Contents

0.1 Introduction

[Abramowitz and Stegun, 1964]

0.2 The input file

The base parameters. What kind of propagator would you like to use? Only supports Crank Nicolson for now

```
    "propagator": "crank_nicolson"
```

. The math library to do the propagation. Hopefully a native threaded version coming soon. Only suuports PETsc right now.

```
    "math_library": "PETsc"
```

. Time step for propagation:

```
    "time_step": 0.1
```

.

The next object in the input json file is the basis. This specifies parameters for the bspline basis in both the eigen state calculation and for the TDSE

```
"basis": {
    "order": 8,
    "node_sequence": "parabolic",
    "num_nodes": 500,
    "x_min": 0.0,
    "x_max": 300.0,
    "lmax": 30,
    "mmax": 0,
    "ecs_r0": 0.9,
    "ecs_theta": 0.3
}
```

.

. . . . .

Eigen state solver,

```
"eigen_state": {
    "solver": "SLEPC",              // only solver that is supported
    "nmax": 4,                      // how many n-states (minus 1 for each L)
    "lmax": 3,                      // optional, nmax-1 by default, final L
    "lmin": 0,                      // optional, 0 by default, starting L
    "tol": 1e-10,                   // optional, ? by default
    "filename": "Ar.h5",            // basis filename
    "expanding": true               // optionalexpand the basis in *filename*?
}
```

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0.3 Some further examples to get started

Bibliography

[Abramowitz and Stegun, 1964] Abramowitz, M. and Stegun, I. A. (1964). *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*. Dover Publications, Inc., New York.