

visit Jens Nielsen

Linear molecules:

The code reproduces the results in the code by Friedrich and Herschbach

Make unit tests to confirm that this will not change in the future

Symmetric tops:

The code correctly calculates the energy for symmetric top molecules.

However as we split using the Wang transformation we get the wrong crossings.

This can be fixed by splitting in to individual k states before the diagonalization.

This code exists and reproduces the results in the calculations by Marko.

Will make these calculations and save some comparisons with Markos results.

Open questions

- Do we have to handle negative Ms?

We can ignore negative M's for now.

Generally only the sign of $M \cdot K$ matter. So a state $M K$ will be degenerated with $-M -K$ for all M and $K \neq 0$

The negative K's are implemented for asymmetric tops as they are renamed in the Wang transformation. The symmetric top Hamiltonian will have negative K's we just need to use them somehow for symmetric tops.

If we implement symmetric tops we need to think about the sign of K.

To do this we need to handle the id of a negative state and replace the minus sign in the hdf file.

- How do we treat nonparallel tensor of inertia and polarizability?

As is 3-aminophenol

Two ideas of doing this:

Calculate the matrix elements in the polarizability tensor system and transfer to the inertia system.

Calculate using the (non diagonal) polarizability tensor in the inertia system.

Calculating the wavefunction and PDF in 3D space

Basis: Wang functions

In principle, could be expressed in terms of Jacobi polynomials

but not for some (K-M) values, can be circumvented through identities
not necessarily numerically stable for large K, M
(Bretislav has used this methode before)

Marko has done it via hypergeometric series -> will send us;-) must implement python
extension for use

could also check them against Mathematica for some values...

Checked in GSL extension for Wigner d from (J. Underwood) and provided Python
wrapper. (there seems to be problems with this implementation. The k=0 i.e.
Spherical harmonics are wrong)

Fortran implementation of Ad van der Avoird checked in in early oktober.

We also have an fft based implementation checked in

Eigenvectors

Sort them according to some labeling of Wang functions |JKMs>
same order as in the matrix

Expand series in basis

Wavefunction in (x, y, z)

Expand asymmetric top wavefunction with eigenvectors in Wang basis (JKMs)

Calculate ensemble average, using thermal populations or populations read from file.

Plot

Send the 3D PDF to Mayavi and let it create 3D plots or 2D projections.

Can it project on an arbitrary axis? (many good mayavi use examples are
available online)

We have code that uses the code by J. Underwood and Ad van der Avoird to make plots of
individual symmetric top states.

State averaging:

The HDF file format right now is changes to the following:

/param/dipole ...

(This should be per isomer basis)

/J/Ka/Kc/M/Isomer/acfield/energy array

/J/Ka/Kc/M/Isomer/acfield/dcfields array

Test for speed and maybe change to something faster if needed.

jkext_plot_energy and jk_ext_print_energy

Implement control of the Kmax and Mmax to plot --> linear molecules k_max=0

And plotting of effective polarizability i.e. derivative of energy with respect to
field squared.

What to do with the program:

Iodobenzene:

Will try to reproduce the experimental results from JCP and PRL

Extract the PADs for a geometry as close as possible to the experimental one.

Up/total and cos theta.

Investigate the degree of orientation for higher static fields. Should we make a new experimental system that will make higher fields possible.

OCS:

Comparison to experimental results for adiabatic and nonadiabatic orientation and alignment.

Calculate the orientation as a function of the deflection

using the input from Franks deflection simulations.

Compare this to new experimental results.

Benzonitrile:

We can directly calculate this in the experimental geometry used in the 1D experiments.

The 3D experiments cannot be simulated using this code.

Discussion:

Jens, Marko, Frank

$M = 0$ --> there is full Wang symmetry, even in field --> implement and test
this is checked in to the trunk but not tested

Jens + Jochen

Effective polarizability

This should be the derivative of energy with respect to field-squared. Should be implemented in `jkext_plot_energy` and `jk_ext_print_energy`.

Jens, Bretislav, and Jochen

Bretislav will think about the case of non-parallel tensors of inertia and polarizability. He suggests to consult Townse&Schawlow or Zare.

In order to further test the matrix elements, look at

limiting cases (field-free and harmonic libration limits)

this would also help understand why the solution is what it is (hierarchy of states)