SpecTraj - Manual

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1 Theory

SpecTraj calculates a power spectrum ($D(\nu)$ at the frequency ν) from the nuclear velocities according to:

$$D(\nu) = 2\beta \sum_{j=1}^{N_\mathrm{A}} m_j \int dt \, \langle \mathbf{v}_j(\tau)\mathbf{v}_j(\tau+t)\rangle_\tau \exp\{-i2\pi\nu t\}. \tag{1}$$

β is equal to $1/(k_\mathrm{B}T)$ with k_B being the Boltzmann constant and T the absolute temperature. m_j and $\mathbf{v}_j$ denote mass and velocity of the nucleus j, respectively, while N_A is the number of atoms.

2 Usage

Please use SpecTraj as follows:

```
python SpecTraj.py [options] [velocity-files] > output
```

The velocity files should have the following structure:

time $[fs]$	v_x $[\sqrt{\frac{2E_H}{u}}]$	v_y $[\sqrt{\frac{2E_H}{u}}]$	v_z $[\sqrt{\frac{2E_H}{u}}]$	mass $[u]$
⋮	⋮	⋮	⋮	⋮

u is the atomic mass unit and E_H is the Hartree energy. For example:

0.1	0.001	-0.100	0.240	12.000
0.2	0.002	-0.105	0.230	12.000
0.3	0.003	-0.109	0.210	12.000
⋮	⋮	⋮	⋮	⋮

The following options are supported:

Option	*Type*	*Explanation*	*Default*
`-b --start-time`	integer	Start taking data from the ith step	0
`-e --end-time`	integer	Take data until the ith step	10^8
`-n --nreps`	integer	Number of replicas for the spectrum	1
`-b --damping`	string	Use exponential damping: `true` or `false`	`true`
`-f --damping-factor`	double	Exponential factor used in the damping function	1000
`-l --lags`	integer	Reduce number of lags by i in the autocorrelation function	0

The resulting output has the following structure:

Wavenumber $[\mathrm{cm}^{-1}]$	$\mathrm{Re}(D/\beta)$	$\mathrm{Im}(D/\beta)$	$\mathrm{Abs}(D/\beta)$	$\mathrm{Re}(D^2/\beta^2)$
⋮	⋮	⋮	⋮	⋮

3 Examples

1. Generate a power spectrum of water from the velocity files of its three atoms:

   ```
   python SpecTraj.py -d true -f 1000 -n 1 vel_h1.dat vel_h2.dat vel_o.dat > water.dat
   ```

2. Generate a power spectrum of water from three individual trajectories (`a`, `b`, and `c`):

   ```
   python SpecTraj.py -d true -f 1000 -n 3 vel_h1_a.dat vel_h2_a.dat vel_o_a.dat
   vel_h1_b.dat vel_h2_b.dat vel_o_b.dat vel_h1_c.dat vel_h2_c.dat vel_o_c.dat > water.dat
   ```

3. Get atomic power spectra of water:

   ```
   python SpecTraj.py -d true -f 1000 -n 1 vel_h1.dat > spec_h1.dat
   python SpecTraj.py -d true -f 1000 -n 1 vel_h2.dat > spec_h2.dat
   python SpecTraj.py -d true -f 1000 -n 1 vel_o.dat > spec_o.dat
   ```