**decoherence\_times2rates(tau)**

Decoherence rates from decoherence times. Zero decoherence rate for the exactly degenerate states and for the self-decoherence (diagonal elements)

**energy\_gaps(Hvib)**

Absolute values of energy gaps for a single trajectory at every timestep.

**energy\_gaps\_ave(Hvib, itimes, nsteps)**

Absolute values of energy gaps averaged over multiple trajectories at every timestep.

– the number of starting times (initial conditions)

- the number of nuclear trajectories (datasets)

**decoherence\_times(Hvib, verbosity=0)**

Decoherence times and rates for a single trajectory

Here,

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– the number of MD steps in this single trajectory

– are the time-points along the MD trajectory, indexed by the integer subscript for clarity in practical implementation.

**decoherence\_times\_ave\_old(Hvib, itimes, nsteps, verbosity=0)**

**WARNING: this function should not be replaced by the next one!**

Decoherence times and rates based on the averaged energy gap fluctuations (averaged by the magnitude)

Here,

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– the number of starting times (initial conditions)

- the number of nuclear trajectories (datasets)

– the number of MD steps in this single trajectory

– are the time-points along the MD trajectory, indexed by the integer subscript for clarity in practical implementation.

– are the starting time-points of the MD trajectory.

**decoherence\_times\_ave(Hvib, itimes, nsteps, verbosity=0)**

Decoherence times and rates based on the averaged energy gap fluctuations (averaged by the magnitude).

Here,

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– the number of starting times (initial conditions)

- the number of nuclear trajectories (datasets)

– the number of MD steps in this single trajectory

– are the time-points along the MD trajectory, indexed by the integer subscript for clarity in practical implementation.

– are the starting time-points of the MD trajectory.