decoherence_times2rates(tau)

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

$$r_{ij} = \begin{cases} \dfrac{1}{\tau_{ij}}, & if\ \tau_{ij} > 0 \\ 0, otherwise \end{cases}$$

energy_gaps(Hvib)

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

$$\Delta E_{ij}(t) = \left|Hvib_{ii}(t) - Hvib_{jj}(t)\right|$$

energy_gaps_ave(Hvib, itimes, nsteps)

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

$$\Delta E_{ij}(t) = \frac{1}{N_{it}N_{tr}} \sum_{k=1}^{N_{it}} \sum_{n=1}^{N_{tr}} \left|Hvib_{ii}^{n}(t_k + t) - Hvib_{jj}^{n}(t_k + t)\right|$$

N_{it} – the number of starting times (initial conditions)

N_{tr}- the number of nuclear trajectories (datasets)

decoherence_times(Hvib, verbosity=0)

Decoherence times and rates for a single trajectory

$$\tau_{ij} = \begin{cases} \sqrt{\dfrac{12}{5}}\dfrac{1}{\delta E_{ij}} & , \delta E_{ij} > 0 \\ 10^{10}, otherwise \end{cases} \qquad r_{ij} = \begin{cases} \dfrac{1}{\tau_{ij}}, & if\ \tau_{ij} > 0 \\ 0, otherwise \end{cases}$$

Here,

$\delta E_{ij} = \sqrt{\frac{1}{N_{steps}} \sum_{p=1}^{N_{steps}} \left(\Delta E_{ij}(t_p) - \langle \Delta E_{ij} \rangle\right)^2}$,

$\langle \Delta E_{ij} \rangle = \frac{1}{N_{steps}} \sum_{p=1}^{N_{steps}} \Delta E_{ij}(t_p)$,

$\Delta E_{ij}(t_p) = \left|Hvib_{ii}(t_p) - Hvib_{jj}(t_p)\right|$.

N_{steps} – the number of MD steps in this single trajectory

$t_p = p\Delta t$ – 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)

$$\tau_{ij} = \begin{cases} \sqrt{\frac{12}{5}}\frac{1}{\delta E_{ij}} & , \delta E_{ij} > 0 \\ 10^{10}, otherwise \end{cases} \qquad r_{ij} = \begin{cases} \frac{1}{\tau_{ij}}, & if\ \tau_{ij} > 0 \\ 0, otherwise \end{cases}$$

Here,

$\delta E_{ij} = \sqrt{\frac{1}{N_{steps}}\sum_{p=1}^{N_{steps}}\left(\Delta E_{ij}(t_p) - \langle\Delta E_{ij}\rangle\right)^2}$,

$\langle\Delta E_{ij}\rangle = \frac{1}{N_{steps}}\sum_{p=1}^{N_{steps}}\Delta E_{ij}(t_p)$,

$\Delta E_{ij}(t_p) = \frac{1}{N_{it}N_{tr}}\sum_{k=1}^{N_{it}}\sum_{n=1}^{N_{tr}}\left|Hvib_{ii}^{n}(t_k + t_p) - Hvib_{jj}^{n}(t_k + t_p)\right|$.

N_{it} – the number of starting times (initial conditions)

N_{tr}- the number of nuclear trajectories (datasets)

N_{steps} – the number of MD steps in this single trajectory

$t_p = p\Delta t$ – are the time-points along the MD trajectory, indexed by the integer subscript for clarity in practical implementation.

t_k – 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).

$$\tau_{ij} = \begin{cases} \sqrt{\frac{12}{5}}\frac{1}{\delta E_{ij}} & , \delta E_{ij} > 0 \\ 10^{10}, otherwise \end{cases} \qquad r_{ij} = \begin{cases} \frac{1}{\tau_{ij}}, & if\ \tau_{ij} > 0 \\ 0, otherwise \end{cases}$$

Here,

$$\delta E_{ij} = \sqrt{\frac{1}{N_{steps}N_{it}N_{tr}}\sum_{p=1}^{N_{steps}}\sum_{k=1}^{N_{it}}\sum_{n=1}^{N_{tr}}\left(\Delta E_{ij}^{n}\left(t_k + t_p\right) - \langle \Delta E_{ij} \rangle\right)^2},$$

$$\langle \Delta E_{ij} \rangle = \frac{1}{N_{steps}N_{it}N_{tr}}\sum_{p=1}^{N_{steps}}\sum_{k=1}^{N_{it}}\sum_{n=1}^{N_{tr}}\Delta E_{ij}^{n}\left(t_k + t_p\right),$$

$$\Delta E_{ij}^{n}\left(t_k + t_p\right) = \left|Hvib_{ii}^{n}\left(t_k + t_p\right) - Hvib_{jj}^{n}\left(t_k + t_p\right)\right|.$$

N_{it} – the number of starting times (initial conditions)

N_{tr}- the number of nuclear trajectories (datasets)

N_{steps} – the number of MD steps in this single trajectory

$t_p = p\Delta t$ – are the time-points along the MD trajectory, indexed by the integer subscript for clarity in practical implementation.

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