MANUAL

SHARC-MN – version 1.0
Surface Hopping with Arbitrary Couplings – MN extension

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SHARC-MN – version 1.0 is built on SHARC – version 2.1.
For recent versions of SHARC, see https://sharc-md.org

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Licensing

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Acknowledgments

We requested permission from the authors of SHARC – version 2.1 to distribute this modified version of the code, and we were given the OK. We are grateful to the authors of SHARC – version 2.1 for making their code available and for their cooperation every step of the way. Some of the modifications in SHARC-MN are scheduled to be included in a future version of SHARC itself.

Our work on the MN extension of SHARC – version 2.1 was supported in part by the U. S. Department of Energy, Office of Basic Energy Sciences.

Citations

Users of SHARC-MN – version 1.0 are requested to cite both SHARC and SHARC-MN. Examples of appropriate referencing are as follows:

- Y. Shu, L. Zhang, and D. G. Truhlar, SHARC-MN – version 1.0 (University of Minnesota, Minneapolis, 2020), https://comp.chem.umn.edu/fcband

See also the references for methods in Sections I.D and I.E.
I. Introduction

SHARC-MN is an extended version of SHARC. Both codes are used for direct dynamics calculations of electronically nonadiabatic processes in which all needed energies, gradients, and nonadiabatic couplings (NACs) are calculated by performing electronic structure calculations as they are needed in the dynamics calculations.

When molecules and materials are electronically excited, the nuclear motion is affected. Processes involving more than one electronic state are called electronically nonadiabatic dynamics. The SHARC and SHARC-MN codes are used for semiclassical simulation of nonadiabatic dynamical processes, i.e., for computing where nuclei move and how electronic coefficients change and decohere. Within the semiclassical approach, one typically treats the nuclei as undergoing classical motion on an effective potential or as classical motion that switches between two or more potentials, while in either case the electrons are treated quantum mechanically with the nuclear and electronic propagations being coupled. There are two categories of methods:

- trajectory surface hopping (TSH): nuclei are propagated at any one time on a single potential energy surface (PES) that is created by electronic structure, and the PES is switched stochastically from time-to-time as the probability of being in different electronic states changes; this switch is called a “hop”. We refer the readers to the SHARC manual (https://sharc-md.org/?page_id=15) for detailed information about using SHARC or SHARC-MN for TSH calculations.
- methods based on a self-consistent potential (SCP): nuclei are propagated on a mean-field PES. These methods are in SHARC-MN but not (at this time) in SHARC, and they are described in this manual. SHARC-MN includes three methods of this type:
  - semiclassical Ehrenfest (SE),
  - coherent switching with decay of mixing (CSDM)
  - self-consistent decay of mixing (SCDM)

The NACs that are usually used for direct dynamics do not conserve angular momentum or the center of mass. SHARC-MN corrects this problem by using a projection operator to remove the translational and rotational components of the originally computed NACs.

The implementation of CSDM, SE, and NAC projection, and the incorporation of adaptive time steps are the major extensions of SHARC that are included in SHARC-MN.

I.A. Introduction to semiclassical Ehrenfest and CSDM

Semiclassical Ehrenfest is similar to surface hopping in that the nuclear wave packet motion is approximated by classical trajectories. However, in contrast to surface hopping, the nuclei in semiclassical Ehrenfest dynamics are propagated on a self-consistent potential. One obtains the self-consistent potential by averaging the PESs over the electronic states considered with weights given by the electronic density matrix.

The advantages of semiclassical Ehrenfest dynamics are:

- The method is derived from the time-dependent Schrödinger equation by a self-consistent field approximation. Employing the self-consistent potential is a natural way to simulate the unitary (fully coherent) motion in which the wave function is a linear combination involving multiple electronic states.[1]
- Employing the self-consistent potential makes semiclassical Ehrenfest dynamics invariant with respect to the choice of electronic-state representation, which may be either adiabatic states or diabatic.

- As in the original surface hopping method, the propagation of the classical trajectories only requires local information about the PESs and couplings, and the nuclear equations of motion follow Newtonian mechanics (although the motion is coupled to electronic motion in a way that has no classical analog).

However, semiclassical Ehrenfest dynamics is notoriously bad for long-time propagation as the trajectory may propagate on unphysical averaged PESs after leaving a strong interaction region, e.g., a region with locally avoided crossing of adiabatic PESs. This poor behavior is due to the lack of decoherence:[2,3,4] in molecules and materials, the electronic density matrix is a reduced density matrix for the electronic subsystem embedded in a “bath” of nuclei, and the nuclear motion causes decoherence of the electronic density matrix. Decoherence causes the density matrix to tend to a diagonal form in an environmentally selected basis called the pointer basis. The robustness of semiclassical Ehrenfest dynamics with respect to the choice of representation is important because in general one does not know which representation (adiabatic, diabatic, or something else) is closest to the pointer basis.[5,6]

The CSDM method adds non-Markovian decoherence to the semiclassical Ehrenfest method so that the electronic coherences (i.e., the off-diagonal elements of the electronic density matrix) decay to zero in the assumed pointer basis after one leaves a region of strongly coupled potential energy surfaces.[4,7] \textit{SHARC-MN} assumes that the pointer basis is the adiabatic one; this is a reasonable assumption for most molecular systems. As a consequence, a CSDM trajectory propagates on a single PES in a pure adiabatic state in asymptotic regions or other regions far from strong interaction regions.

\textit{SHARC-MN} can also do calculations by semiclassical decay of mixing (SCDM) [3]. The SCDM method, like SE and CSDM, is a self-consistent potential method, and it may be considered an older version of CSDM with a less accurate (but simpler) treatment of decoherence. We recommend CSDM over SCDM because it is more accurate, and therefore we de-emphasize SCDM in the manual. The user who is interested in SCDM (for historical reasons or because it is simpler) should note, however, that any option that is available for CSDM is also available for SCDM.

**I.B. Important note**

To understand \textit{SHARC-MN}, users must read original \textit{SHARC} manual. This manual only has descriptions of methods and keywords that are added to the \textit{SHARC} code.
I.C. New features in SHARC-MN – version 1.0 (additions to SHARC – version 2.1):
These features are new in SHARC-MN – version 1.0 (2020):

- Dynamics program *sharc.x*:
  - New methods: semiclassical Ehrenfest dynamics, CSDM (coherent switching with decay of mixing, which adds non-Markovian decoherence to semiclassical Ehrenfest), and SCDM (older, less accurate version of CSDM)
  - New versions of semiclassical Ehrenfest, CSDM, and SCDM dynamics based on overlap (time-derivative couplings).
  - Adaptive time-step propagation: adaptive Velocity Verlet or Bulirsch-Stoer
  - Projected NAC for conserving of nuclear angular momentum and the center of mass in direct dynamics with TSH, semiclassical Ehrenfest, CSDM, or SCDM
- Data extraction:
  - New options in *data_extractor.x*
- Auxiliary scripts:
  - *setup_traj.py* works for setting up both surface hopping and self-consistent potential methods, where the self-consistent potential method may be SE, CSDM, or SCDM.

I.D. References: basic methods
The following references may be cited for the basic methods in SHARC-MN:


In addition, users may cite the references in section I.E for specific dynamical methods.

I.E. References: specific methods

- semiclassical Ehrenfest (SE): [8,9]
- coherent switching with decay of mixing (CSDM): [8]
- SE and CSDM by using time derivative couplings: [10]
- Projected NAC: [11]

I.F. Installation
Install of SHARC-MN requires the system specific modification of *Makefile* that is located in the source folder. Installation is done by a single command from the source folder:

```
make
```

The SHARC-MN executable is *sharc.x*; the output data extractor is called *data_extractor.x*. 
II. Input Keywords

II.A. List of keywords

Table II.1: Input keywords for sharc.x. The first column gives the name of the keyword, the second lists possible arguments, and the third line provides an explanation. Defaults are marked in green like this. $n$ denotes the n-th argument to the keyword.

The table gives keywords that are new or have new options in SHARC-MN as compared to SHARC. (The overlap keyword has not changed, but it is included for completeness.) Users should refer to Table 4.1 in original SHARC manual for other keywords.

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Arguments</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>method</td>
<td>string</td>
<td>Set the simulation method.</td>
</tr>
<tr>
<td></td>
<td>$1=tsh$</td>
<td>Use trajectory surface hoping (TSH).</td>
</tr>
<tr>
<td></td>
<td>$1=scp$, ehrenfest</td>
<td>Use a self-consistent potential scheme (SE, CSDM, or SCDM). Either $1=scp$ or $1=ehrenfest$ will use a self-consistent potential; these two choices of keyword have the same meaning. Note that CSDM and SCDM are both combinations of Ehrenfest with decay of mixing and pointer-state switching.</td>
</tr>
<tr>
<td>nsubsteps</td>
<td>integer</td>
<td>Number of substeps for the integration of the electronic equation of motion.</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>This is equal to the ratio of the step size for integrating the nuclear equations of motion to the step size for integrating the electronic equations.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>It is recommended to use a large number of substeps (e.g., 200) when performing SE and CSDM.</td>
</tr>
<tr>
<td>coupling</td>
<td>string</td>
<td>Quantities describing the nonadiabatic couplings.</td>
</tr>
<tr>
<td></td>
<td>$1=ddr$, nacdr</td>
<td>Uses vectorial nonadiabatic couplings $\langle \psi_I</td>
</tr>
<tr>
<td></td>
<td>$2=ddt$, nacdt</td>
<td>Uses temporal nonadiabatic couplings $\langle \psi_I</td>
</tr>
<tr>
<td></td>
<td>$3=overlap$</td>
<td>Uses the overlaps $\langle \psi_I (t_0)</td>
</tr>
<tr>
<td>decoherence_scheme</td>
<td>string</td>
<td>Method for decoherence correction.</td>
</tr>
<tr>
<td></td>
<td>$1=none$</td>
<td>No decoherence correction.</td>
</tr>
<tr>
<td></td>
<td>$1=edc$</td>
<td>Energy-difference-based correction for TSH. The TSH/EDC scheme is explained in Refs. [12,13] and is based on an earlier approximation [4] to the decoherence time in terms of energy gaps and nuclear kinetic energies.</td>
</tr>
<tr>
<td></td>
<td>$1=afssh$</td>
<td>Augmented FSSH for TSH (refer to original SHARC manual for details of augmented FSSH)</td>
</tr>
<tr>
<td></td>
<td>$1=dom$</td>
<td>Add decay-of-mixing decoherence terms to SE to perform CSDM or SCDM.</td>
</tr>
<tr>
<td>switching_procedure</td>
<td>string</td>
<td>Method for scheme used to switch the pointer state in decay-of-mixing calculations</td>
</tr>
<tr>
<td></td>
<td>$1=csdm$</td>
<td>Coherent switching with decay of mixing [4,8]</td>
</tr>
<tr>
<td></td>
<td>$1=scdm$</td>
<td>Self-consistent decay of mixing [3,8]</td>
</tr>
</tbody>
</table>
### II.B. Detailed description of the keywords

#### method
The `method` keyword controls the method to be used for dynamics

- `tsh` for trajectory surface hopping
- `scp` for methods with self-consistent potentials, which are SE, CSDM, and SCDM).

To run CSDM, which is recommended, set `method` to `scp` and `decoherence_scheme` to `dom`.

#### integrator
The `integrator` keyword controls the integrator to be used in dynamics

- `fvv` for fixed time step Velocity Verlet
- `avv` for adaptive time step Velocity Verlet,
- `bsh` for Bulirsch-Stoer integrator

The `fvv` integrator is same as the default integrator in previous `SHARC` programs. We recommend using `fvv` or `avv`.

#### convthre
The `convthre` keyword controls the maximum allowed differences between successive time steps in adaptive integrators. For `avv`, it is the maximum allowed energy difference in the current and previous time steps.

#### dtmin
The `dtmin` keyword controls the minimum allowed time step for adaptive integrators.
**decoherence_scheme**
When performing self-consistent potential based methods, the decoherence is introduced with the decay-of-mixing algorithm. Use of the decay-of-mixing decoherence scheme is turned on by setting `decoherence_scheme dom`. The other two options, i.e. `decoherence_scheme edc` and `decoherence_scheme afssh`, are used for calculations with the trajectory surface hopping method.

**switching procedure**
There are two options for the computation of the probabilities of switching pointer states in the decay-of-mixing algorithms, and they can be set with the `switching_procedure` keyword.

- `switching_procedure csdm` turns on coherent switching with decay of mixing [4,8], which is the default and is recommended.
- `switching_procedure scdm` turns on the older self-consistent decay of mixing [3,8]

**neom**
The `neom` keyword is used to control the form of the nonadiabatic coupling vector in the nuclear equations of motion; note that this is a separate choice from the form of the NAC used in the electronic equations of motion. One can directly use the nonadiabatic coupling vector by using either `neom nacdr` or `neom ddr`; this will require using an electronic structure theory code to compute the nonadiabatic coupling vector. Alternatively, one can use an effective nonadiabatic coupling vector by setting `neom gdiff`. The effective nonadiabatic coupling vector is a vector defined in Section IV.C as a combination of the difference gradient vector and the velocity vector. The dot product between the effective nonadiabatic coupling vector and velocity vector equals the overlap of electronic wave functions at successive steps. See reference [10] for detailed description of effective nonadiabatic coupling vector. Using the effective nonadiabatic coupling vector is the default option if one uses time-derivative coupling to propagate electronic coefficients, which is set by `coupling overlap`. If one uses `neom gdiff`, one must use `coupling overlap`, and if one uses `coupling overlap` one may use `neom nacdr`, `neom nacdr`, or `neom gdiff`.

**nac_projection** and **nonac_projection**
This two keywords control the use of projected nonadiabatic coupling vector or original nonadiabatic coupling vector. The projected nonadiabatic coupling vector conserves nuclear angular momentum and the center of mass, and is the recommended choice; it is also the default. We refer readers to reference [11] for detailed description of projection operator.
II.C. Combinations of keywords

Possible combinations of the keywords are shown in Table II.2.

**Table II.2:** Possible combinations of **coupling**, **neom**, and **nac_projection** keywords for running SE or CSDM calculations

<table>
<thead>
<tr>
<th>keywords</th>
<th>nuclear EOM</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>nardr(ddr) nardr(ddr) nac_projection</td>
<td>eq 21</td>
<td>The method used in refs. [8,11]</td>
</tr>
<tr>
<td>nardr(ddr) nardr(ddr) nonac_projection</td>
<td>eq 9</td>
<td></td>
</tr>
<tr>
<td>overlap nardr(ddr) nac_projection</td>
<td>eq 21</td>
<td>recommended to be most accurate</td>
</tr>
<tr>
<td>overlap nacdr(ddr) nonac_projection</td>
<td>eq 9</td>
<td></td>
</tr>
<tr>
<td>overlap gdiff nac_projection</td>
<td>eq 10</td>
<td>The method used in ref. [10]</td>
</tr>
<tr>
<td>overlap gdiff nonac_projection</td>
<td>eq 17</td>
<td></td>
</tr>
</tbody>
</table>

*All three keywords are used in all of the self-consistent-potential methods.*
III. Output

SHARC provides an auxiliary program data_extractor.x, which can operate on the output.dat file to extract properties as a function of time along the trajectory. We refer the users to Table 7.5 and Section 7.10 Data Extractor: data_extractor.x in original SHARC manual for a detailed description of the data_extractor.x program. Here we describe additional options for this program.

Table III.1. Additional command-line options for data_extractor.x.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
<th>Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>-h</td>
<td>Display help message and quit.</td>
<td>Help not displayed</td>
</tr>
<tr>
<td>-f</td>
<td>File name</td>
<td>None – file name must be given.</td>
</tr>
<tr>
<td>-sk</td>
<td>skip parsing of geom., vel., grad., NAC.</td>
<td>False</td>
</tr>
<tr>
<td>-ccd</td>
<td>Write coeff_diag.out</td>
<td>False</td>
</tr>
<tr>
<td>-dend</td>
<td>Write density_diag.out</td>
<td>False</td>
</tr>
<tr>
<td>-cdend</td>
<td>Write edensity_diag.out</td>
<td>False</td>
</tr>
<tr>
<td>-denm</td>
<td>Write density_mch.out</td>
<td>False</td>
</tr>
<tr>
<td>-rdd</td>
<td>Write den_state_diag.out</td>
<td>True</td>
</tr>
<tr>
<td>-crdd</td>
<td>Write eden_state_diag.out</td>
<td>False</td>
</tr>
<tr>
<td>-rdm</td>
<td>Write den_state_mch.out</td>
<td>True</td>
</tr>
</tbody>
</table>

- xs -e, -rdm, -rdd, -d, -cd, -cm, -p, -x
- s -ccd, -sp, -xm, -cb, -da plus -xs Default
- l -crdd, -id, -im, plus -s
- xl -ccd, -dend, -cdend, -denm, plus -l
Table III.2. Content of the files written by `data_extractor.x` corresponding to the additional options shown in Table III.1.

- $n$ is the total number of states.
- $j$ is a state index ($j \in \{1, \ldots, n\}$).

<table>
<thead>
<tr>
<th>File</th>
<th>#Columns</th>
<th>Columns</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ccoeff_diag.out</td>
<td>$2 + 2n$</td>
<td>1</td>
<td>Time: $t$ (fs)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Norm of coherent wave function:</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\sum_j</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$1 + 2j$ Re$\left[c_{j,\text{coherent}}^{\text{diag}}\right]$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$2 + 2j$ Im$\left[c_{j,\text{coherent}}^{\text{diag}}\right]$</td>
</tr>
<tr>
<td>density_diag.out</td>
<td>$1+(n+1)^*/2$</td>
<td>1</td>
<td>Time: $t$ (fs)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Density matrix element $D_{ij}$ in the diagonal representation</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$1+n^*(j-1)+k-j+1$</td>
</tr>
<tr>
<td>cdensity_diag.out</td>
<td>$1+(n+1)^*/2$</td>
<td>1</td>
<td>Time: $t$ (fs)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Coherent density matrix element $D_{ij}^{\text{coherent}}$ in the diagonal</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>representation.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$1+n^*(j-1)+k-j+1$</td>
</tr>
<tr>
<td>density_mch.out</td>
<td>$1+(n+1)^*/2$</td>
<td>1</td>
<td>Time: $t$ (fs)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Density matrix element $D_{ij}$ in the MCH representation</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$1+n^*(j-1)+k-j+1$</td>
</tr>
<tr>
<td>den_state_diag.out</td>
<td>$1+n$</td>
<td>1</td>
<td>Time $t$ (fs)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Real diagonal density matrix element $\text{Re}\left[D_{ii}\right]$ in the</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>diagonal representation</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$n$</td>
</tr>
<tr>
<td>cden_state_diag.out</td>
<td>$1+n$</td>
<td>1</td>
<td>Time $t$ (fs)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Real diagonal coherent density matrix element $\text{Re}\left[D_{ii}^{\text{coherent}}\right]$ in the diagonal representation.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$n$</td>
</tr>
<tr>
<td>den_state_mch.out</td>
<td>$1+n$</td>
<td>1</td>
<td>Time $t$ (fs)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Real diagonal density matrix element $\text{Re}\left[D_{ii}\right]$ in the</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>MCH representation</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$n$</td>
</tr>
</tbody>
</table>
IV. Theory

IV.A. Decoherence by decay of mixing

Decay of mixing is described in Refs. [2,3,4,8]. We refer the reader to Ref. [8] for details of implementing decay of mixing to be compatible with SHERC; the decoherent propagator is introduced in the MCH representation. The decay-of-mixing decoherence scheme is used by decoherence_scheme.dom. The electronic coefficients are propagated with the following electronic equation of motion:

\[
\mathbf{c}_{\text{diag}}(t+\tau) = \mathbf{U}(t+\tau)\mathbf{P}_C^{\text{MCH}}(t,\tau)\mathbf{P}_D^{\text{MCH}}(t,\tau)\mathbf{U}(t)\mathbf{c}_{\text{diag}}(t)
\]

(1)

The coherent propagator and decoherent propagator (which is diagonal) are

\[
\mathbf{P}_C^{\text{MCH}}(t+\Delta t,\tau) = \exp\left(-\left(i\mathbf{H}^{\text{MCH}} + \mathbf{v} \cdot \mathbf{d}^{\text{MCH}}\right)\Delta t\right)
\]

(2)

\[
\left[\mathbf{P}_D^{\text{MCH}}(t+\Delta t,\tau)\right]_{II} = \begin{cases} 
-\frac{\Delta t}{2\tau_I(t)} & I \neq K \\
\sum_{J=K}^{N} \frac{\Delta t}{2\tau_J(t)} \rho_{JJ}^{\text{MCH}}(t) & I = K
\end{cases}
\]

(3)

where \(\tau_I\) is the decoherence time for state \(I\):

\[
\tau_I = \frac{\hbar}{|V_I - V_K|}\left(C + \frac{2E_0}{\sum_{i}^{N_{\text{atoms}}} M_i |v_i \cdot \hat{s}_{i,IK}|^2}\right)
\]

(4)

where \(V_I\) is the adiabatic energy of state \(I\), and

\[
\hat{s}_{i,IK} = \frac{s_{i,IK}}{|s_{i,IK}|}
\]

(5)

where \(C\) and \(E_0\) are parameters, and \(M_i\) and \(v_i\) are the mass and velocity of atom \(i\). The default values of the parameters are \(C = 1\) (unitless) and \(E_0 = 0.1\) hartree. The decoherent direction \(s_{IK}\) is given by,

\[
s_{IK} = \text{Re}\left(\frac{d_0 P_{\text{vib}} \cdot d_{IK}}{|d_{IK}|} d_{IK}\right) + P_{\text{vib}}
\]

(6)

where \(a_0 = 1\) bohr, \(P_{\text{vib}}\) is the internal vibrational momentum (computed by removing the overall angular motion from the total momentum of the molecule), and \(d_{IK}\) is the nonadiabatic coupling vector between state \(I\) and decoherent state \(K\). We use “decoherent state” and “pointer state” as synonyms.

IV.B. Pointer-state switching

The CSDM pointer-state switching probabilities between decoherent state \(K\) and another state \(I\) is,
\[ P_{K \rightarrow I} = \left( 1 - \left[ c_{K}^{\text{diag}} (t + \Delta t) \right]_{\text{co}}^2 \right) \]

\[ \times \left[ c_{K}^{\text{diag}} (t) \right]_{\text{co}}^2 \left( c_{K}^{\text{diag}} (t + \Delta t) \right)_{IK}^\ast \left( c_{K}^{\text{diag}} (t) \right)_{IK}^\ast \]

where \( c_{K}^{\text{diag}} (t) \) are the coherent coefficients propagated fully coherently along the trajectory, and they are reset to \( c_{K}^{\text{diag}} (t) \) at each local minimum \( D_K \). The coupling strength \( D_K \) is defined differently depend on which coupling is used. For nonadiabatic coupling vector,

\[ D_K (t) = \sum_{l \neq K} |d_{lk}| \quad (8) \]

For overlap,

\[ D_K (t) = \sum_{l \neq K} |\sigma_{IK}| \quad (9) \]

Using of equation 9 is similar to the CSDM-C version in original CSDM reference[4]. The keyword coupling controls the use of equation 8 or 9 automatically, equation 8 corresponds to coupling \( \text{ddr} \) or coupling \( \text{nacdr} \), and equation 9 corresponds to coupling \( \text{overlap} \). The negative switching probabilities are set to zero and

\[ P_{K \rightarrow K} = 1 - \sum_{l \neq K} P_{K \rightarrow l} \quad (10) \]

We refer the reader to reference [8] for details. This is used with \text{switching\_procedure csdm}.

**IV.C. Effective nonadiabatic coupling**

The nuclear equation of motion in self-consistent potential methods in its original form requires full information of nonadiabatic couplings:

\[ \dot{P}(t) = -\sum_l \text{Re} (\rho_{II}) \frac{\partial V_l}{\partial R} + \sum_l \sum_{j \neq l} \text{Re} (\rho_{lI}) (V_l - V_j) d_{lj} \]

One can, however, employs an effective nonadiabatic couplings, \( G_{lI} \) to replace \( d_{lj} \). Using of \( G_{lI} \) requires eq 9 to be re-written as,

\[ \dot{P} = -\sum_l \text{Re} (\rho_{II}) \frac{\partial V_l}{\partial R} + \sum_l \sum_{j \neq l} \left[ \frac{\text{Re} (\rho_{lI}) (V_l - V_j) \sigma_{lj}}{v \cdot G_{lI}} \right] G_{lI} \]

The \( G_{lI} \) is defined as,

\[ G_{lI} = g_{lI} + \alpha \hat{R} \]

where \( \alpha \) is a parameter defined as

\[ \alpha = \frac{\sigma_{lj} - \hat{R} \cdot g_{lj}}{\hat{R} \cdot \hat{R}} \]

\[ (11) \]

\[ (12) \]
A consequence of eq 24 is that
\[
\dot{\mathbf{R}}(t) \cdot \mathbf{G}_{ij}(t) = \sigma_{ij}(t)
\]  
(13)
where,
\[
\sigma_{ij}(t) = \langle \dot{\phi}_i(r; \mathbf{R}(t)) | \dot{\phi}_j(r; \mathbf{R}(t)) \rangle / \partial t
\]
(14)
is time-derivative coupling. This is related to a nonadiabatic coupling by,
\[
\sigma_{ij}(t) = \dot{\mathbf{R}}(t) \cdot \mathbf{d}_{ij}(t)
\]  
(15)
And comparison of eq 13 to eq 15 justifies calling \( \mathbf{G}_{ij} \) an effective nonadiabatic coupling. To preserve the angular momentum, one should use a projected effective nonadiabatic coupling,
\[
\mathbf{G}_{ij}^Q = (1 - \mathbf{Q}) (\mathbf{g}_{ij} + \alpha \dot{\mathbf{R}})
\]
(16)
where \( \mathbf{Q} \) is a projection operator that removes translational and rotational components. And hence using of a projected effective nonadiabatic coupling results in the nuclear equation of motion as,
\[
\ddot{\mathbf{P}} = -\sum_{i} \text{Re}(\rho_{ij}) \frac{\partial V_I}{\partial \mathbf{R}} + \sum_{i} \sum_{j \neq i} \left[ \frac{\text{Re}(\rho_{ij})(V_i - V_j) \sigma_{ij}}{\mathbf{v} \cdot \mathbf{G}_{ij}^Q} \right] \mathbf{G}_{ij}^Q
\]
(17)
Setting \text{nem ddr} and \text{nem nacdr} is using eq 9 to propagate the nuclear equation of motion, while setting \text{nem gdiff} is using eq 10 or 17 to propagate the nuclear equation of motion depends on whether one sets \text{nonac_projection} or \text{nac_projection}.

**IV.D. Projection operator**
To conserve both the nuclear angular momentum and the center of mass in nonadiabatic dynamics trajectories with TSH or self-consistent potential methods, one should use the projected nonadiabatic coupling or the projected effective nonadiabatic coupling.

The projection operator is a \( 3N \times 3N \) matrix with elements
\[
Q_{i\alpha,i'\alpha'} = \frac{1}{N} \delta_{\alpha\alpha'} + \sum_{\beta} \sum_{\beta'} \sum_{\gamma \gamma'} \epsilon_{\alpha \beta \gamma} R_{\alpha \beta} [\mathbf{\hat{I}}^{-1}]_{\beta \beta'} \sum_{\gamma'} \epsilon_{\alpha' \beta' \gamma'} R_{\gamma' \gamma} Q_{i \gamma,i' \gamma'}
\]
(18)
where indices \( i \) and \( i' \) label the nuclei and vary from 1 to \( N \), \( \alpha, \beta, \gamma, \alpha', \beta', \) and \( \gamma' \) take on the values \( x, y, \) and \( z \), \( \mathbf{\hat{I}}^{-1} \) is the inverse of matrix \( \mathbf{\hat{I}} \), matrix \( \mathbf{\hat{I}} \) is same as moment of inertia matrix with all masses set to 1, and \( \epsilon \) is the completely antisymmetric third-order unit pseudotensor, whose elements are the Levi-Civita symbol. The first term of the projection operator projects onto the three directions corresponding to overall translation, and the second term projects onto the three directions corresponding to overall rotation.

Use of projection operator on nonadiabatic coupling results in a projected nonadiabatic coupling,
\[
\mathbf{d}_{ij}^Q = (1 - \mathbf{Q}) \mathbf{d}_{ij}
\]
(19)
For TSH, one uses the projected NAC when the momentum after a hop is adjusted,
\[
\mathbf{P}_{\text{post-hop}} = \mathbf{P}_{\text{pre-hop}} - \alpha_{ij} \mathbf{d}_{ij}^Q
\]
(20)
For semiclassical Ehrenfest and CSDM dynamics, one employs a self-consistent potential (SCP), and this yields...
\[
\mathbf{P} = -\sum_{I=1}^{n} \text{Re}(\rho_{II}) \frac{\partial V_I}{\partial \mathbf{R}} + \sum_{I=1}^{n} \sum_{J \neq I}^{n} \left[ \text{Re}(\rho_{IJ})(V_I - V_J) \frac{(\mathbf{v} \cdot \mathbf{d}_{IJ})}{\mathbf{v} \cdot \mathbf{d}_{IJ}^Q} \right] \mathbf{d}_{IJ}^Q
\]

(21)

For CSDM, the decoherent direction is,

\[
\mathbf{s}_{AK} = a_{0} \mathbf{P}_{\text{vib}} \cdot \frac{\mathbf{d}_{AK}^Q}{|\mathbf{d}_{AK}^Q|} \mathbf{d}_{AK}^Q + \mathbf{P}_{\text{vib}}
\]

(22)

We refer users to reference [11] for more detailed information.
V. References


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Version 3, 29 June 2007

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