PyCCE

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GETTING STARTED

CHAPTER

ONE

THEORETICAL BACKGROUND

This document contains a brief list of the coupling parameters between the central and the bath spins used in **PyCCE**, a description of the qubit dephasing, and a summary of the cluster correlation expansion (CCE) method. You can find more details in the following references[1][2][3].

1.1 Hamiltonian

The **PyCCE** package allows one to simulate the dynamics of a central spin or multiple central spins interacting with a spin bath through the following Hamiltonian:

$$\hat{H} = \hat{H}_S + \hat{H}_{SB} + \hat{H}_B$$

Where $\hat{H}_S$ is the Hamiltonian of the free central spin or several spins, $\hat{H}_{SB}$ denotes interactions between central spin and a spin belonging to the bath, and $\hat{H}_B$ are intrinsic bath spin interactions. For a single central spin, this corresponds to the following Hamiltonian:

$$\begin{aligned}
\hat{H}_S &= \mathbf{S}\mathbf{D}\mathbf{S} + \mathbf{B}\gamma_S\mathbf{S} \\
\hat{H}_{SB} &= \sum_i \mathbf{S}\mathbf{A}_i\mathbf{I}_i \\
\hat{H}_B &= \sum_i \mathbf{I}_i\mathbf{P}_i\mathbf{I}_i + \mathbf{B}\gamma_i\mathbf{I}_i + \sum_{i<j} \mathbf{I}_i\mathbf{J}_{ij}\mathbf{I}_j
\end{aligned}$$

Where $\mathbf{S} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ are the components of spin operators of the central spin, $\mathbf{I} = (\hat{I}_x, \hat{I}_y, \hat{I}_z)$ are the components of the bath spin operators, and $\mathbf{B} = (B_x, B_y, B_z)$ is an external applied magnetic field.

If several central spins are considered, the central spin Hamiltonian is modified as following:

$$\hat{H}_S = \sum_i (\mathbf{S_i}\mathbf{D_i}\mathbf{S_i} + \mathbf{B}\gamma_{S_i}\mathbf{S_i} + \sum_{i<j} \mathbf{S_i}\mathbf{K_{ij}}\mathbf{S_j})$$

And the spin-bath Hamiltonian is equal to the following:

$$\hat{H}_{SB} = \sum_{i,j} \mathbf{S}_i\mathbf{A}_{ij}\mathbf{I}_j$$

The interactions are described by the following tensors that are either required to be input by user or can be generated by the package itself (see *Hamiltonian Parameters Input* for details):

[1] Mykyta Onizhuk and Giulia Galli. "PyCCE: A Python Package for Cluster Correlation Expansion Simulations of Spin Qubit Dynamic". Adv. Theory Simul. 2021, 2100254, https://onlinelibrary.wiley.com/doi/10.1002/adts.202100254

[2] Wen Yang and Ren-Bao Liu. "Quantum many-body theory of qubit decoherence in a finite-size spin bath". Phys. Rev. B78, p. 085315, https://link.aps.org/doi/10.1103/PhysRevB.78.085315

[3] Mykyta Onizhuk et al. "Probing the Coherence of Solid-State Qubits at Avoided Crossings". PRX Quantum 2, p. 010311. https://link.aps.org/doi/10.1103/PRXQuantum.2.010311.

- $\mathbf{D}$ ($\mathbf{P}$) is the self-interaction tensor of the central spin (bath spin). For the electron spin, the tensor corresponds to the zero-field splitting (ZFS) tensor. For nuclear spins corresponds to the quadrupole interactions tensor.
- γ_i‘‘is the magnetic field interaction tensor of the :math:‘i-spin describing the interaction of the spin and the external magnetic field B.
- $\mathbf{A}$ is the interaction tensor between central and bath spins. In the case of the nuclear spin bath, it corresponds to the hyperfine couplings.
- $\mathbf{J}$ is the interaction tensor between bath spins.
- $\mathbf{K}$ is the interaction tensor between central spins.

1.2 Qubit dephasing

Usually, two coherence times are measured to characterize the loss of a qubit coherence - T_1 and T_2. T_1 defines the timescale over which the qubit population is thermalized; T_2 describes a purely quantum phenomenon - the loss of the phase of the qubit's superposition state.

In the pure dephasing regime ($T_1 >> T_2$) the decoherence of the central spin is completely determined by the decay of the off diagonal element of the density matrix of the qubit.

Namely, if the qubit is initially prepared in the $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\phi}|1\rangle)$ state, the loss of the relative phase of the $|0\rangle$ and $|1\rangle$ levels is characterized by the coherence function:

$$\mathcal{L}(t) = \frac{\langle 1|\,\hat{\rho}_S(t)\,|0\rangle}{\langle 1|\,\hat{\rho}_S(0)\,|0\rangle} = \frac{\langle\hat{\sigma}_-(t)\rangle}{\langle\hat{\sigma}_-(0)\rangle}$$

Where $\hat{\rho}_S(t)$ is the density matrix of the central spin and $|0\rangle$ and $|1\rangle$ are qubit levels.

The cluster correlation expansion (CCE) method was first introduced in ref.[Page 1, 2]. The core idea of the CCE approach is that the spin bath-induced decoherence can be factorized into set of irreducible contributions from the bath spin clusters. Written in terms of the coherence function:

$$\mathcal{L}(t) = \prod_C \tilde{L}_C = \prod_i \tilde{L}_{\{i\}} \prod_{i,j} \tilde{L}_{\{ij\}} \cdots$$

Where each cluster contribution is defined recursively as:

$$\tilde{L}_C = \frac{L_C}{\prod_{C'} \tilde{L}_{C' \subset C}}$$

Where L_C is a coherence function of the qubit, interacting only with the bath spins in a given cluster C (with the cluster Hamiltonian $\hat{H}_C$), and $\tilde{L}_{C'}$ are contributions of C' subcluster of C.

For example, the contribution of the single spin i is equal to the coherence function of the bath with one isolated spin i:

$$\tilde{L}_i = L_i$$

The contribution of pair of spins i and j is equal to:

$$\tilde{L}_{ij} = \frac{L_{ij}}{\tilde{L}_i \tilde{L}_j}$$

and so on.

Maximum size of the cluster included into the expansion determines the order of CCE approximation. For example, in the CCE2 approximation, only contributions up to spin pairs are included, and in CCE3 - up to triplets of bath spins are included, etc.

The way the coherence function for each cluster is computed slightly varies between depending on whether the conventional or generalized CCE method is used.

In the case of the several central spins, one can apply CCE formalism to compute any off-diagonal element of the combined density matrix.

1.2.1 Conventional CCE

In the original formulation of the CCE method, the total Hamiltonian of the system is reduced to the sum of two effective Hamiltonians, conditioned on the qubit levels of the central spin:

$$\hat{H} = 00 \otimes \hat{H}^{(0)} + 11 \otimes \hat{H}^{(1)}$$

Where $\hat{H}^{(\alpha)}$ is an effective Hamiltonian acting on the bath when the central spins are in the α state ($\alpha = 0, 1$ is one of the two eigenstates of the $\hat{H}_S$ chosen as qubit levels).

Given an initial qubit state $\psi = \frac{1}{\sqrt{2}}(0 + e^{i\phi}1)$ and an initial state of the bath spin cluster C characterized by the density matrix $\hat{\rho}_C$, the coherence function of the qubit interacting with the cluster C is computed as:

$$L_C(t) = Tr[\hat{U}_C^{(0)}(t)\hat{\rho}_C\hat{U}_C^{(1)\dagger}(t)]$$

Where $\hat{U}_C^{(\alpha)}(t)$ is time propagator defined in terms of the effective Hamiltonian $\hat{H}_C^{(\alpha)}$ and the number of decoupling pulses. Note that $\hat{H}_C^{(\alpha)}$ here includes only degrees of freedom of the given cluster.

For free induction decay (FID) the time propagators are trivial:

$$\hat{U}_C^{(0)} = e^{-\frac{i}{\hbar}\hat{H}_C^{(0)}t};\ \hat{U}_C^{(1)} = e^{-\frac{i}{\hbar}\hat{H}_C^{(1)}t}$$

And for the generic decoupling sequence with N (even) decoupling pulses applied at $t_1, t_2 ... t_N$ we write:

$$\hat{U}^{(\alpha)}(t) = e^{-\frac{i}{\hbar}\hat{H}_C^{(\alpha)}(t_N - t_{N-1})}e^{-\frac{i}{\hbar}\hat{H}_C^{(\beta)}(t_{N-1} - t_{N-2})}...e^{-\frac{i}{\hbar}\hat{H}_C^{(\beta)}(t_2 - t_1)}e^{-\frac{i}{\hbar}\hat{H}_C^{(\alpha)}t_1}$$

Where $\alpha = 0, 1$ and $\beta = 1, 0$ accordingly (when $\alpha = 0$ one should take $\beta = 1$ and vice versa). $t = \sum_i t_i$ is the total evolution time. In sequences with odd number of pulses *N*, the leftmost propagator is the exponent of $\hat{H}_C^{(\beta)}$.

1.2.2 Generalized CCE

Instead of projecting the total Hamiltonian on the qubit levels, one may directly include the central spin degrees of freedom to each clusters. We refer to such formulation as gCCE.

In this case we write the cluster Hamiltonian as:

$$\hat{H}_C = \hat{H}_S + \sum_{k,i\in C}\mathbf{S}_k\mathbf{A}_{ki}\mathbf{I}_i + \sum_{i\in C}\mathbf{I}_i\mathbf{P}_i\mathbf{I}_i + \mathbf{B}\gamma_i\mathbf{I}_i + \sum_{i<j\in C}\mathbf{I}_i\mathbf{J}_{ij}\mathbf{I}_j + \sum_{k,a\notin C}\mathbf{S}_k\mathbf{A}_{ka}\langle\mathbf{I}_a\rangle + \sum_{i\in C,\ a\notin C}\mathbf{I}_i\mathbf{J}_{ia}\langle\mathbf{I}_a\rangle$$

And the coherence function of the cluster $L_C(t)$ is computed as:

$$L_C(t) = 0\hat{U}_C(t)\hat{\rho}_{C+S}\hat{U}_C^{\dagger}(t)1$$

Where $\hat{\rho}_{C+S} = \hat{\rho}_C \otimes \hat{\rho}_S$ is the combined initial density matrix of the bath spins' cluster and central spins.

Further details on the theoretical background are available in the references below.

CHAPTER

TWO

QUICK START

The generic workflow of the simulation includes first the generation of the spin bath in the material, and second carrying the CCE dynamics calculations for the qubit interacting with this spin bath.

2.1 Base Units

- All coupling constants are given in kHz.
- Timesteps are in millisecond (ms).
- Distances are in angstrom (A).
- Gyromagnetic ratios are given in $\mathrm{rad} \cdot \mathrm{ms}^{-1} \cdot \mathrm{G}^{-1}$.
- Quadrupole constants are given in barn ($10^{-28}\ \mathrm{m}^2$).
- Magnetic field is given in Gauss (G).

2.2 Simple Example

The simplest example includes the following steps:

1. Generate the `BathCell` object. Here we use the interface with `ase` which can effortlessly generate unit cells of many materials. As an example, we import the diamond structure.

```
import numpy as np
import pycce as pc
from ase.build import bulk

cell = pc.BathCell.from_ase(bulk('C', 'diamond', cubic=True))
```

2. Using the `BathCell` object, generate spin bath of the most common isotopes in the material. Here we generate the spin bath of size 200 Angstrom and remove one carbon, where the spin of interest is located, from the diamond crystal lattice.

```
atoms = cell.gen_supercell(200, remove=('C', [0, 0, 0]))
```

   This function returns the `BathArray` instance, which contains names of the bath spins in `'N'`, their coordinates in angstrom in `'xyz'`, empty arrays of hyperfine couplings in kHz in `'A'`, and quadrupole couplings in kHz in `'Q'` namefields. The hyperfine couplings will be generated by `Simulator` in the next step. For alternative ways to define hyperfine couplings see *Hamiltonian Parameters Input*.

3. Setup the `Simulator` using the generated spin bath. The first required argument `spin` is the total spin of the central spin or the `CenterArray` instance, containing properties of the central spins. `r_bath`, `r_dipole` and `order` are convergence parameters (see the *Tutorials* for examples of convergence), `magnetic_field` is the external applied magnetic field along the z-axis, and `pulses` is the number of decoupling π pulses in Carr-Purcell-Meiboom-Gill (CPMG) sequence or a more complicated sequence, set with `Pulse` objects.

   ```
   calc = pc.Simulator(0.5, position=[0, 0, 0], bath=atoms, r_bath=40,
                       r_dipole=6, order=2, magnetic_field=500, pulses=1)
   ```

   The hyperfine couplings are automatically generated at this step assuming point dipole-dipole interactions between central spin and bath spins.

4. Compute the coherence function of the qubit using `.compute` method of the `Simulator` object with conventional CCE.

   ```
   time_points = np.linspace(0, 2, 101)
   coherence = calc.compute(time_points)
   ```

This function outputs Numpy array with the same shape as the `time_points` and contains the coherence function computed at each time step. By default `compute` method uses the conventional CCE to compute the coherence function.

More detailed examples of **PyCCE** usage are available in the tutorials.

CHAPTER

THREE

TUTORIALS

The examples below are available as Jupyter notebooks in the Github repository.

3.1 NV Center in Diamond

In this tutorial we will go over the main steps of running CCE calculations for the NV center in diamond with the **PyCCE** module. Those include:

- Generating the spin bath using the `pycce.BathCell` instance.
- Setting up properties of the `pycce.Simulator` instance.
- Running the calculations with the `Simulator.compute` function.

We will compute the Hahn-echo coherence function (with decoupling π-pulse applied) using the following available methods:

- Conventional CCE.
- Generalized CCE (gCCE).
- gCCE with Monte-Carlo bath sampling.

Finally, we will run a simulation on how different bath polarization will impact Hahn-echo signal.

```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

import sys
import pycce as pc
import ase

from mpl_toolkits import mplot3d

seed = 8805
np.random.seed(seed)
np.set_printoptions(suppress=True, precision=5)
```

3.1.1 Generate nuclear spin bath

Building a supercell of nuclear spins from the `ase.Atoms` object.

Build BathCell

To generate cell it from `ase.atoms` object, use classmethod `BathCell.from_ase`.

```
from ase.build import bulk

# Generate unitcell from ase
diamond = bulk('C', 'diamond', cubic=True)
diamond = pc.read_ase(diamond)
```

The following attributes are created with this initiallization:

- `.cell` is ndarray containing information of lattice vectors. Each **column** is a lattice vector in cartesian coordinates.
- `.atoms` is a dictionary with keys corresponding to the atom name, and each item is a list of the coordinates in cell coordinates.

```
print('Cell\n', diamond.cell)
print('\nAtoms\n', diamond.atoms)
```

```
Cell
 [[3.57 0.   0.  ]
 [0.   3.57 0.  ]
 [0.   0.   3.57]]

Atoms
 defaultdict(<class 'list'>, {'C': [array([0., 0., 0.]), array([0.25, 0.25, 0.25]),␣
↪array([0. , 0.5, 0.5]), array([0.25, 0.75, 0.75]), array([0.5, 0. , 0.5]), array([0.75,
↪ 0.25, 0.75]), array([0.5, 0.5, 0. ]), array([0.75, 0.75, 0.25])]})
```

Populate BathCell with isotopes

The **PyCCE** package uses EasySpin database of the concentrations of all common stable isotopes with non-zero spin, however the user can proide custom concentrations.

Use function `BathCell.add_isotopes` to add one (or several) isotopes of the element. Each isotope is initiallized with `tuple` containing name of the isotope and its concentration.

Name of the isotope includes the number and element symbol, provided in the `atoms` object. As an output, the `BathCell.add_isotopes` method returns view on dictionary `BathCell.isotopes` which can be modified directly. Structure of the dictionary-like object:

```
{element_1: {isotope_1: concentration, isotope_2: concentration},
 element_2: {isotope_3: concentration ...}}
```

```
# Add types of isotopes
diamond.add_isotopes(('13C', 0.011))
```

```
defaultdict(dict, {'C': {'13C': 0.011}})
```

Isotopes may also be directly added to `BathCell.isotopes`. For example, below we are adding an isotope without the nuclear spin:

```
diamond.isotopes['C']['14C'] = 0.001
```

Set z-direction of the bath (optional)

In the `Simulator` object everything is set in S_z basis. When the quantization axis of the defect does not allign with the (0, 0, 1) direction of the crystal axis, the user needs to define the axis.

If one wants to specify the complete rotation of cartesian axes, one can provide a rotation matrix to rotate the cartesian reference frame with respect to the cell coordinates by calling the `BathCell.rotate` method.

```
# set z direction of the defect
diamond.zdir = [1, 1, 1]
```

Generate spin bath

To generate the spin bath, use the `BathCell.gen_supercell` method. First argument is the linear size of the supercell (minimum distance between any two faces of the supercell is equal to or larger than this parameter). Additional keyword arguments are `remove` and `add`.

`remove` takes a `tuple` or `list of tuples` as an argument. First element of each tuple is the name of the **atom** at that location, second element - coordinates in unit cell coordinates. If such atoms are found in the supercell, they are removed from it.

`add` takes a `tuple` or `list of tuples` as an argument. First element of each tuple is the name of the **isotope** at that location, second element - coordinates in unit cell coordinates. Each of the specified isotopes will be added in the final supercell at specified locations.

```
# Add the defect. remove and add atoms at the positions (in cell coordinates)
atoms = diamond.gen_supercell(200, remove=[('C', [0., 0, 0]),
                                           ('C', [0.5, 0.5, 0.5])],
                              add=('14N', [0.5, 0.5, 0.5]),
                              seed=seed)
```

```
/home/onizhuk/midway/codes_development/pyCCE/pycce/bath/array.py:222: UserWarning: Spin␣
↪type for 14C was not provided and was not found in common isotopes.
  obj[n] = array[n]
```

Note, that because the `14C` isotope doesn't have a spin, **PyCCE** does not find it in common isotopes, and raises a warning. We have to provide `SpinType` for it separately, or define the properties as follows:

```
atoms['14C'].gyro = 0
atoms['14C'].spin = 0
```

3.1.2 BathArray Structure

The bath spins are stored in the `BathArray` object - a subclass of `np.ndarray` with fixed datastructure:

- `N` field `dtype('<U16')` contains the names of bath spins.
- `xyz` field `dtype('<f8', (3,))` contains the positions of bath spins (in A).
- `A` field `dtype('<f8', (3, 3))` contains the hyperfine coupling of bath spins (in kHz).
- `Q` field `dtype('<f8', (3, 3))` contains the quadrupole tensor of bath spins (in kHz) (Relevant for spin >= 1).

All of the fields are accesible as attributes of `BathArray`. Additionally, the subarrays of the specific spins are accessible with their name as indicated above.

Upon generation of the array from the cell, the `Q` and `A` fields are empty. The Hyperfine couplings will be automatically computed by the `Simulator` object, however the quadrupole couplings must be set by the user.

The additional attributes allow one to access `SpinType` properties:

- `name` returns the spin name or array of spin names;
- `spin` returns the value of the spin or array of ones;
- `gyro` returns gyromagnetic ratios of the spins;
- `q` returns quadrupole constants of the spins;
- `h` returns a dictionary with user-defined additions to the Hamiltonian.
- `detuning` returns detunings of the spins (See definition below).

For example, below we print out the attributes of the first two spins in the `BathArray`.

```
print('Names\n', atoms[:2].N)
print('\nCoordinates\n', atoms[:2].xyz)
print('\nHyperfine tensors\n', atoms[:2].A)
print('\nQuadrupole tensors\n',atoms[:2].Q)
```

```
Names
 ['13C' '13C']

Coordinates
 [[-13.97678  -1.48178 -92.75132]
 [ 27.89939  42.17939 -45.86038]]

Hyperfine tensors
 [[[0. 0. 0.]
  [0. 0. 0.]
  [0. 0. 0.]]

 [[0. 0. 0.]
  [0. 0. 0.]
  [0. 0. 0.]]]

Quadrupole tensors
 [[[0. 0. 0.]
  [0. 0. 0.]
  [0. 0. 0.]]

 [[0. 0. 0.]
```

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```
  [0. 0. 0.]
  [0. 0. 0.]]]
```

The properties of spin types (gyromagnetic ratio, quadrupole moment, etc) are stored in the `BathArray.types` attribute, which is an instance of `SpinDict` containing `SpinType` classes. For most known isotopes `SpinType` can be found in the `pycce.common_isotopes` dictionary, and is set by default (including electron spin-1/2, which is denoted by setting `N = e`). The user can add additional `SpinType` objects, by calling `BathArray.add_type` method or setting elements of `SpinDict` directly. For details of the first approach see documentation of `SpinDict.add_type` method.

The direct setting of types is rather simple. The user can set elements of `SpinDict` with `tuple`, containing:

- **(spin, gyromagnetic ratio, quadrupole moment (optional), detuning (optional),)**

  OR

- **(isotope, spin, gyromagnetic ratio, quadrupole moment (optional), detuning (optional),)**

where:

- **isotope** (*str*) is the name of the given spin (same one as in `N` field of `BathArray`) to define new `SpinType` object. The key of `SpinDict` **has** to be the correct name of the spin ("isotope" field in the tuple).
- **spin** (*float*) is the total spin of the given bath spin.
- **gyromagnetic ratio** (*float*) is the gyromagnetic ratio of the given bath spin.
- **quadrupole moment** (*float*) is the quadrupole moment of the given bath spin. Relevant only when electric field gradient are used to generate quadrupole couplings for spins, stored in the `BathArray`, with `BathArray.from_efg` method.
- **detuning** (float) is an additional energy splitting for model spins, included as an extra $+\omega\hat{S}_z$ term in the Hamiltonian, where ω is the detuning.

Units of gyromagnetic ratio are rad / ms / G, quadrupole moments are given in barn, detunings are given in kHz.

```
# Several ways to set SpinDict elements
atoms.types['14C'] = 0, 0, 0
atoms.types['Y'] = ('Y', 0, 0, 0)
atoms.types['A'] = pc.SpinType('A', 0, 0, 0)

print(atoms.types)
```

```
SpinDict(13C: (0.5, 6.7283), 14N: (1.0, 1.9338, 0.0204), 14C: (0.0, 0.0000), ...)
```

3.1.3 Simulator class

The parameters of the CCE simulator engine.

Main parameters to consider:

- `spin` — Either instance of the `CenterArray` or float - total spin of the central spin (assuming one central spin).
- `bath` — spin bath in any specified format. Can be either:
  - Instance of `BathArray` class;
  - `ndarray` with `dtype([('N', np.unicode_, 16), ('xyz', np.float64, (3,))])` containing names of bath spins (same ones as stored in self.ntype) and positions of the spins in angstroms;
  - The name of the `.xyz` text file containing 4 columns: name of the bath spin and xyz coordinates in A.

- `r_bath` — cutoff radius around the central spin for the bath.
- `order` — maximum size of the cluster.
- `r_dipole` — cutoff radius for the pairwise distance to consider two nuclear spins to be connected.
- `magnetic_field` — applied magnetic field. Can also be provided during the simulation run.
- `pulses` — number of pulses in Carr-Purcell-Meiboom-Gill (CPMG) sequence or the pulse sequence itself.

For the full description see the documentation of the `Simulator` object.

First we setup a "mock" instance of `Simulator` to visualize the smaller part of the bath around the central spin.

```
# Setting the runner engine
mock = pc.Simulator(spin=1, position=[0,0,0],
                    bath=atoms, r_bath=20,
                    r_dipole=6, order=3)
```

During the initiallization, depending on the provided keyword arguments several methods may be called:

- `Simulator.read_bath` is called if keyword `bath` is provided. It may take several additional arguments:
  - `r_bath` - cutoff distance from the qubit for the bath.
  - `skiprows` - if `bath` is provided as `.xyz` file, this argument tells how many rows to skip when reading the file.
  - `external_bath` - `BathArray` instance, which contains bath spins with pre defined hyperfines to be used.
  - `hyperfine` - defines the way to compute hyperfine couplings. If it is not given and `bath` doesn't contain any predefined hyperfines (`bath['A'].any() == False`) the point dipole approximation is used. Otherwise it can be an instance of `pc.Cube` object, or callable with signature `func(coord, gyro, central_gyro)`, where `coord` is an array of the bath spin coordinate, gyro is the gyromagnetic ratio of bath spin, central_gyro is the gyromagnetic ratio of the central bath spin.
  - `types` - instance of `SpinDict` or input to create one.
  - `error_range` - maximum allowed distance between positions in `bath` and `external_bath` for two spins to be considered the same.
  - `ext_r_bath` - cutoff distance from the qubit for the `external_bath`. Useful if `external_bath` has very assymetric shape and user wants to keep the precision level of the hyperfine at different distances consistent.
  - `imap` - instance of the `pc.InteractionMap` class, which contain tensor of bath spin interactions. If not provided, interactions between bath spins are assumed to be the same as one of point dipoles.

  Generates `BathArray` object with hyperfine tensors to be used in the calculation.
- `Simulator.generate_clusters` is called if `order` and `r_dipole` are provided. It produces `dict` object, which contains the indexes of the bath spins in the clusters.

  We implemented the following procedure to determine the clusters:

  Each bath spin i forms a cluster of one. Bath spins i and j form cluster of two if there is an edge between them (distance $d_{ij} \leq$ `r_dipole`). Bath spins i, j, and k form a cluster of three if enough edges connect them (e.g., there are two edges ij and jk) and so on. In general, we assume that spins $\{i..n\}$ form clusters if they form a connected graph. Only clusters up to the size indicated by the `order` parameter (equal to CCE order) are included.

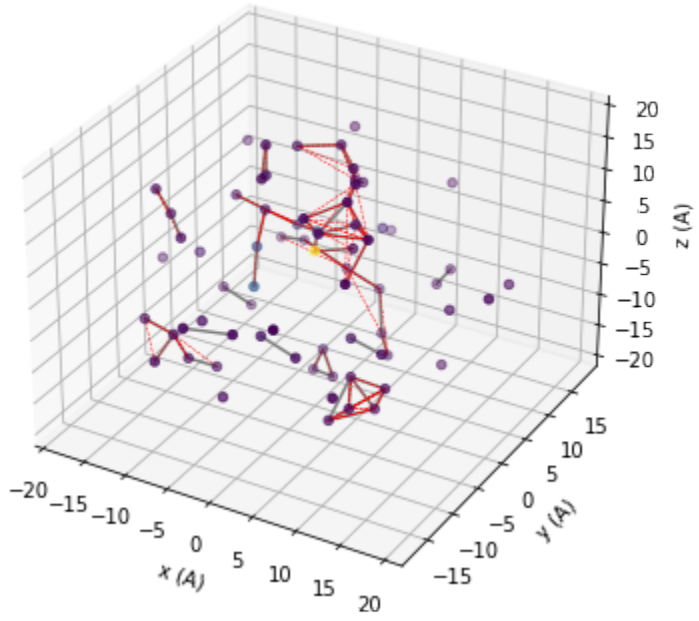
We use `matplotlib` to visualize the spatial distribution of the spin bath. The grey lines show connected pairs of nuclear spins, red dashed lines show clusters of three. You can try to increase `r_dipole`, `r_bath` parameters, or increase `order` and visuallize.

```
# add 3D axis
fig = plt.figure(figsize=(6,6))
ax = fig.add_subplot(projection='3d')

# We want to visualize the smaller bath
data = mock.bath

# First plot the positions of the bath
colors = np.abs(data.A[:,2,2]/data.A[:,2,2].max())
ax.scatter3D(data.x, data.y, data.z, c=colors, cmap='viridis');
# Plot all pairs of nuclear spins, which are contained
# in the calc.clusters dictionary under they key 2
for c in mock.clusters[2]:
    ax.plot3D(data.x[c], data.y[c], data.z[c], color='grey')
# Plot all triplets of nuclear spins, which are contained
# in the calc.clusters dictionary under they key 3
for c in mock.clusters[3]:
    ax.plot3D(data.x[c], data.y[c], data.z[c], color='red', ls='--', lw=0.5)

ax.set(xlabel='x (A)', ylabel='y (A)', zlabel='z (A)');
```



Now we setup `Simulator` object for the actual simulation.

```
# Parameters of CCE calculations engine

# Order of CCE aproximation
order = 2
# Bath cutoff radius
r_bath = 40  # in A
# Cluster cutoff radius
r_dipole = 8  # in A
```

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We will use the `CenterArray` object to store the properties of the central spin, however for simple usecases one can provide the corresponding keywords to the `Simulator` object directly (see examples below).

```
# position of central spin
position = [0, 0, 0]
# Qubit levels (in Sz basis)
alpha = [0, 0, 1]; beta = [0, 1, 0]
# ZFS Parametters of NV center in diamond
D = 2.88 * 1e6 # in kHz
E = 0 # in kHz
nv = pc.CenterArray(spin=1, position=position, D=D, E=E, alpha=alpha, beta=beta)
```

The code already knows the properties of the most common nuclear spins and of elecron spin (accessible under the name `'e'`), however the user can provide their own by calling `BathArray.add_type` method. The way to initiallize `SpinType` objects is the same as in `SpinDict` above.

```
# The code already knows most exsiting isotopes.
#              Bath spin types
#              name    spin    gyro       quadrupole (for s>1/2)
spin_types = [('14N',  1,      1.9338,    20.44),
              ('13C',  1 / 2,  6.72828),
              ('29Si', 1 / 2, -5.3188),]
atoms.add_type(*spin_types)
```

Setting the `Simulator` object

All of the kwargs can be provided at the moment of creation. If all of the kwargs are provided, several methods of the `Simulator` class are called:

- `Simulator.read_bath`;
- `Simulator.generate_clusters`.

The details are available in the `Simulator` methods description.

```
# Setting the runner engine
calc = pc.Simulator(spin=nv, bath=atoms,
                    r_bath=r_bath, r_dipole=r_dipole, order=order)
```

Taking advantage of subclassing `np.ndarray` we can change *in situ* the quadrupole tensor of the Nitrogen nuclear spin.

```
nspin = calc.bath
# Set model quadrupole tensor at N atom
quad = np.asarray([[-2.5, 0, 0],
                   [0, -2.5, 0],
                   [0, 0,  5.0]]) * 1e3 * 2 * np.pi

nspin['Q'][nspin['N'] == '14N'] = quad
```

Note, that we need to apply the boolean mask **second** because of how structured arrays work.

Compute coherence function with conventional CCE

The general interface to compute any property with PyCCE is implemented through the `Simulator.compute` method. It takes two keyword arguments to determine which quantity to compute and how:

- `method` can take 'cce' or 'gcce' values, and determines which method to use - conventional or generalized CCE.
- `quantity` can take 'coherence' or 'noise' values, and determines which quantity to compute - coherence function or autocorrelation function of the noise.

Each of the methods can be performed with Monte Carlo bath state sampling (if `nbstates` keyword is non zero) and with interlaced averaging (If `interlaced` keyword is set to `True`).

In the first example we use the conventional CCE method without Monte Carlo bath state sampling. In the conventional CCE method the Hamiltonian is projected on the qubit levels, and the coherence is computed from the overlap of the bath evolution, entangled with two different qubit states.

The conventional CCE requires one argument:

- `timespace` — time points at which the coherence function is computed.

Additionally, one can provide the following arguments now, instead of when initiallizing `Simulator` object:

- `pulses` — number of pulses in CPMG sequence (0 - FID, 1 - HE etc., default 0) or explicit sequence of pulses as `Sequence` class instance.
- `mangetic_field` — magnetic field along z-axis or vector of the magnetic field. Default (0, 0, 0).

```
# Time points
time_space = np.linspace(0, 2, 201)  # in ms
# Number of pulses in CPMG seq (0 = FID, 1 = HE)
n = 1
# Mag. Field (Bx By Bz)
b = np.array([0, 0, 500])  # in G

l_conv = calc.compute(time_space, pulses=n, magnetic_field=b,
                      method='cce', quantity='coherence', as_delay=False)
```

```
%%timeit
calc.compute(time_space, pulses=n, magnetic_field=b,
             method='cce', quantity='coherence', as_delay=False)
```

```
705 ms ± 9.74 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

Generalized CCE (gCCE)

In contrast to the conventional CCE method, in generalized CCE arpproach each cluster includes the central spin explicitly.

`Simulator` can take `pulses` argument as an actual pulse sequence with an iterable of `Pulse` objects.

For example:

```
p1 = pc.Pulse('x', np.pi)
p2 = pc.Pulse('y', np.pi)
seq = [p1, p2, p1, p2]
```

`seq` will define XY-4 pulse sequence.

An integer number to define the number of pulses is also accepted as in the case of conventional CCE. If the integer is provided, the code assumes the CPMG sequence.

```
# Hahn-echo pulse sequence
pulse_sequence = [pc.Pulse('x', np.pi)]

# Calculate coherence function
l_generatilze = calc.compute(time_space, magnetic_field=b,
                             pulses=pulse_sequence,
                             method='gcce', quantity='coherence')
```

```
%%timeit
calc.compute(time_space, magnetic_field=b,
             pulses=pulse_sequence,
             method='gcce',
             quantity='coherence')
```

```
1.92 s ± 24.6 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

gCCE with random sampling of bath states

Using this approach, one may carry out generalized CCE calculations for the set of random bath states. This functionality can be turned on by by setting the keyword argument `nbstates` to a number of bath states to sample over. Recommended number of bath states is above 100, but the convergence should be checked for each system. Note, that this computation is roughly `nbstates` times longer than an equivalent generalized CCE calculation, as it computes everything `nbstates` times.

For details see `help(calc.compute)`.

```
# Number of random bath states to sample over
n_bath_states = 20

# Calculate coherence function
l_gcce = calc.compute(time_space, magnetic_field=b,
                      pulses=pulse_sequence,
                      nbstates=n_bath_states,
                      method='gcce', quantity='coherence', seed=seed)
```

```
%%timeit
n_bath_states = 5
calc.compute(time_space, magnetic_field=b,
             pulses=pulse_sequence,
             nbstates=n_bath_states,
             method='gcce', quantity='coherence', seed=seed)
```

```
11.9 s ± 379 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

Take a look at the results of three different methods, and check that they produce similar coherence decay. Note that the results obtained using gCCE with bath states sampling deviates from other ones (generalized and conventional CCE), as the chosen number of states (20) is not enough to converge.

```
plt.plot(time_space, l_conv.real,
         label='conventional CCE')
```

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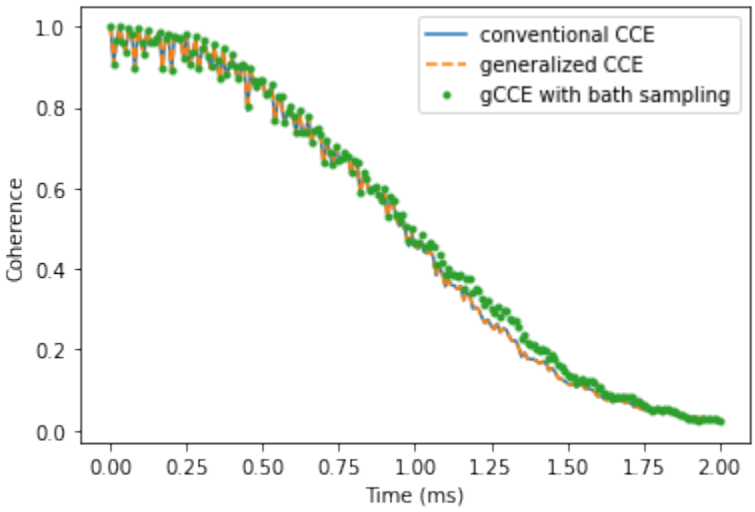
```
plt.plot(time_space, l_generatilze.real,
         label='generalized CCE', ls='--')
plt.plot(time_space, l_gcce.real,
         label='gCCE with bath sampling', ls='', marker='.')
plt.legend()
plt.xlabel('Time (ms)')
plt.ylabel('Coherence');
```



3.1.4 Convergence parameters

Having confirmed that all methods produce the same results, we check the convergence of the conventional CCE with respect to `order`, `r_bath`, `r_dipole` parameters of the `Simulator` object.

First, define all of the parameters.

```
parameters = dict(
    order=2, # CCE order
    r_bath=40,  # Size of the bath in A
    r_dipole=8,  # Cutoff of pairwise clusters in A
    position=[0, 0, 0], # Position of central Spin
    alpha=[0, 0, 1],
    beta=[0, 1, 0],
    pulses = 1, # N pulses in CPMG sequence
    magnetic_field=[0,0,500]
) # Qubit levels)

time_space = np.linspace(0, 2, 201)  # Time points in ms
```

We can define a little helper function to streamline the process. Note that resetting the parameters automatically recomputes the properties of the bath.

```
def runner(variable, values):
    invalue = parameters[variable]
    calc = pc.Simulator(spin=1, bath=atoms, **parameters)
```

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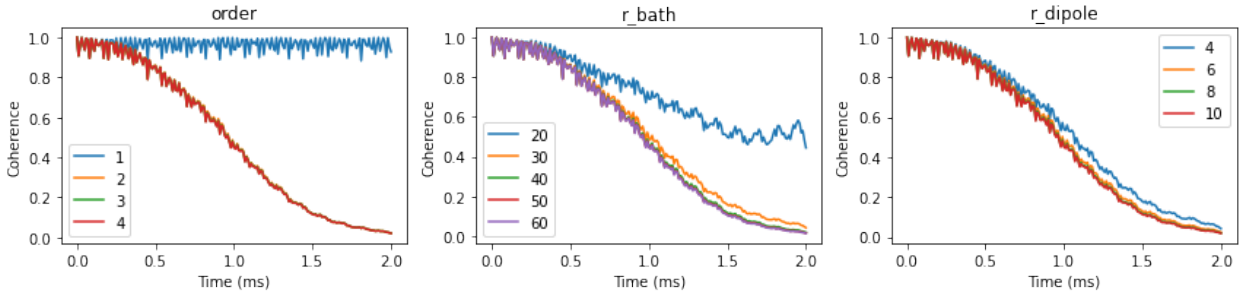
```
    ls = []

    for v in values:
        setattr(calc, variable, v)
        l = calc.compute(time_space, method='cce',
                         quantity='coherence')

        ls.append(l.real)

    parameters[variable] = invalue
    ls = pd.DataFrame(ls, columns=time_space, index=values).T
    return ls
```

Now we can compute the coherence function at different values of the parameters:

```
orders = runner('order', [1, 2, 3, 4])
rbs = runner('r_bath', [20, 30, 40, 50, 60])
rds = runner('r_dipole', [4, 6, 8, 10])
```

We can visualize the convergence of the coherence function with respect to different parameters:

```
fig, axes = plt.subplots(1, 3, figsize=(12, 3))
orders.plot(ax=axes[0], title='order')
rbs.plot(ax=axes[1], title='r_bath')
rds.plot(ax=axes[2], title='r_dipole')
for ax in axes:
    ax.set(xlabel='Time (ms)', ylabel='Coherence')
fig.tight_layout()
```



3.1.5 Bath polarization

To study different bath polarization we will modify `BathArray.state` attribute, which contains spin states for each bath spin. For simplicity we will assume the gaussian profile of the polarization.

```
def polarize(bath, gamma=5):
    # Polarizations of each bath spin
    if gamma > 0:
        polos = np.exp(-(bath.dist()/gamma)**2) * 0.5
    else:
        polos = np.zeros(bath.size)
```

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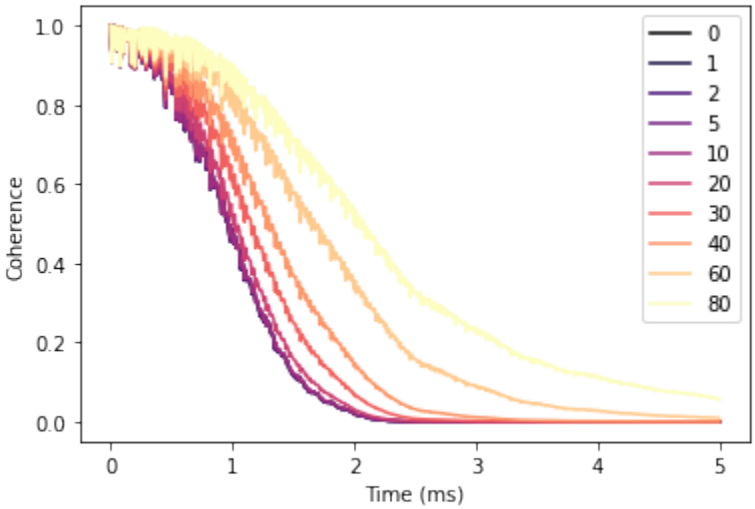
```
    for a, pol in zip(bath, polos):

        # Skip 14N
        if a.N != '13C':
            continue
        # Generate density matrix
        dm = np.zeros((2, 2), dtype=np.complex128)
        dm[0,0] = 0.5 + pol
        dm[1,1] = 0.5 - pol
        a.state =  dm

    return

# Use already optimized parameters
calc = pc.Simulator(spin=1, bath=atoms, **parameters)

# Standard deviations of the polarization gaussian profile
gammas = [0, 1, 2, 5, 10, 20, 30, 40, 60, 80]
ls = []

ts = np.linspace(0, 5, 501)
for gamma in gammas:
    polarize(calc.bath, gamma=gamma)
    l = calc.compute(ts)
    ls.append(l.real)

df = pd.DataFrame(ls, columns=ts, index=gammas).T
```

With increased polarization in the bath the Hahn-echo signal decays significantly slower.

```
fig, ax = plt.subplots()
df.plot(cmap='magma', ax=ax)
ax.set(xlabel='Time (ms)', ylabel='Coherence');
```



3.2 VV in SiC

An example of computing Free Induction Decay (FID) and Hahn-echo (HE) with hyperfine couplings from GIPAW for axial and basal divacancies.

```
import numpy as np
import matplotlib.pyplot as plt
import sys
import ase
import pandas as pd
import warnings
import pycce as pc

np.set_printoptions(suppress=True, precision=5)
warnings.simplefilter("ignore")

seed = 8805
```

3.2.1 Axial kk-VV

First we compute FID and HE for axial divacancy.

Build BathCell from the ground

One can set up an `BathCell` instance by providing the parameters of the unit cell, or `cell` argument as 3x3 tensor, where each column defines a, b, c unit cell vectors in cartesian coordinates.

In this tutorial we use the first approach.

```
# Set up unit cell with (a, b, c, alpha, beta, gamma)
sic = pc.BathCell(3.073, 3.073, 10.053, 90, 90, 120, 'deg')
# z axis in cell coordinates
sic.zdir = [0, 0, 1]
```

Next, user has to define positions of atoms in the unit cell. It is done with `BathCell.add_atoms` function. It takes an unlimited number of arguments, each argument is a tuple. First element of the tuple is the name of the atom, second - list of xyz coordinates either in cell units (if keyword `type='cell'`, default value) or in Angstrom (if keyword `type='angstrom'`). Returns `BathCell.atoms` dictionary, which contains list of coordinates for each type of elements.

```
# position of atoms
sic.add_atoms(('Si', [0.00000000, 0.00000000, 0.1880]),
              ('Si', [0.00000000, 0.00000000, 0.6880]),
              ('Si', [0.33333333, 0.66666667, 0.4380]),
              ('Si', [0.66666667, 0.33333333, 0.9380]),
              ('C', [0.00000000, 0.00000000, 0.0000]),
              ('C', [0.00000000, 0.00000000, 0.5000]),
              ('C', [0.33333333, 0.66666667, 0.2500]),
              ('C', [0.66666667, 0.33333333, 0.7500]));
```

Two types of isotopes present in SiC: ^{29}Si and ^{13}C. We add this information with the `BathCell.add_isotopes` function. The code knows most of the concentrations, so this step is actually unnecessary. If no isotopes is provided, the natural concentration of common magnetic isotopes is assumed.

```
# isotopes
sic.add_isotopes(('29Si', 0.047), ('13C', 0.011))

# defect position in cell units
vsi_cell = [0, 0, 0.1880]
vc_cell = [0, 0, 0]

# Generate bath spin positions
atoms = sic.gen_supercell(200, remove=[('Si', vsi_cell),
                                       ('C', vc_cell)],
                          seed=seed)
```

Read Quantum Espresso output

PyCCE provides a helper function `read_qe` in `pycce.io` module to read hyperfine couplings from quantum espresso output. `read_qe` takes from 1 to 3 positional arguments:

- `pwfile` name of the pw input/output file;
- `hyperfine` name of the gipaw output file containing hyperfine couplings;
- `efg` name of the gipaw output file containing electric field tensor calculations.

During its call, `read_qe` will read the cell matrix in pw file and apply it to the coordinates is necessary. However, usually we still need to rotate and translate the Quantum Espresso supercell to allign it with our `BathArray`. To do so we can provide additional keywords arguments `center` and `rotation_matrix`. `center` is the position of (0, 0, 0) point in coordinates of pw file, and `rotation_matrix` is rotation matrix which aligns z-direction of the GIPAW output. This matrix, acting on the (0, 0, 1) in Cartesian coordinates of GIPAW output should produce (a, b, c) vector, alligned with zdirection of the BathCell. Keyword argument `rm_style` shows whether `rotation_matrix` contains coordinates of new basis set as rows (`'row'`, common in physics) or columns (`'col'`, common in math).

```
# Prepare rotation matrix to alling with z axis of generated atoms
# This matrix, acting on the [0, 0, 1] in Cartesian coordinates of GIPAW output
# Should produce [a, b, c] vector, alligned with zdirection of the BathCell
M = np.array([[0, 0, -1],
              [0, -1, 0],
              [-1, 0, 0]])

# Position of (0,0,0) point in cell coordinates
center = [0.6, 0.5, 0.5]
# Read GIPAW results
exatoms = pc.read_qe('axial/pw.in',
                     hyperfine='axial/gipaw.out',
                     center=center, rotation_matrix=M,
                     rm_style='col',
                     isotopes={'C':'13C', 'Si':'29Si'})
```

`pc.read_qe` produces instance of `BathArray`, with names of bath spins as the most common isotopes of the following elements (if keyword `isotopes` set to `None`) or from the mapping provided by the `isotopes` argument.

Set up CCE Simulator

In this example we set up a bare `Simulator` and add properties of the spin bath later.

```
# Setting up CCE calculations
pos = sic.to_cartesian(vsi_cell)
CCE_order = 2
r_bath = 40
r_dipole = 8
B = np.array([0, 0, 500])

calc = pc.Simulator(1, pos, alpha=[0, 0, 1], beta=[0, 1, 0], magnetic_field=B)
```

Function `Simulator.read_bath` can be called explicitly to initiallize spin bath. Additional keyword argument `external_bath` takes instance of `BathArray` with hyperfine couplings read from Quantum Espresso. The program then finds the spins with the same name at the same positions (within the range defined by `error_range` keyword argument) in the total bath and sets their hyperfine couplings.

Finally, we call `Simulator.generate_clusters` to find the bath spin clusters in the provided bath.

```
calc.read_bath(atoms, r_bath, external_bath=exatoms);
calc.generate_clusters(CCE_order, r_dipole=r_dipole);
```

FID with DFT hyperfine couplings

We provide `pulses` argument directly to the compute function instead of during initiallization of the `Simulator` object.

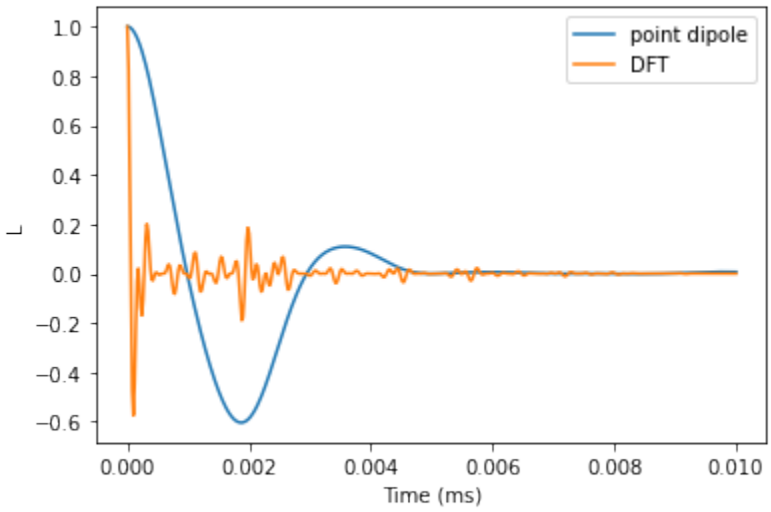
```
time_space = np.linspace(0, 0.01, 501)
N = 0

ldft = calc.compute(time_space, pulses=N, as_delay=False)
```

FID with hyperfine couplings from point dipole approximation

```
pdcalc = pc.Simulator(1, pos, alpha=[0, 0, 1], beta=[0, 1, 0], magnetic_field=B,
                      bath=atoms, r_bath=r_bath, order=CCE_order, r_dipole=r_dipole)
lpd = pdcalc.compute(time_space, pulses=N, as_delay=False)
```

Plot the results and and verify that the predictions are significantly different.

```
plt.plot(time_space, lpd.real, label='point dipole')
plt.plot(time_space, ldft.real, label='DFT')
plt.legend()
plt.xlabel('Time (ms)')
plt.ylabel('L');
```



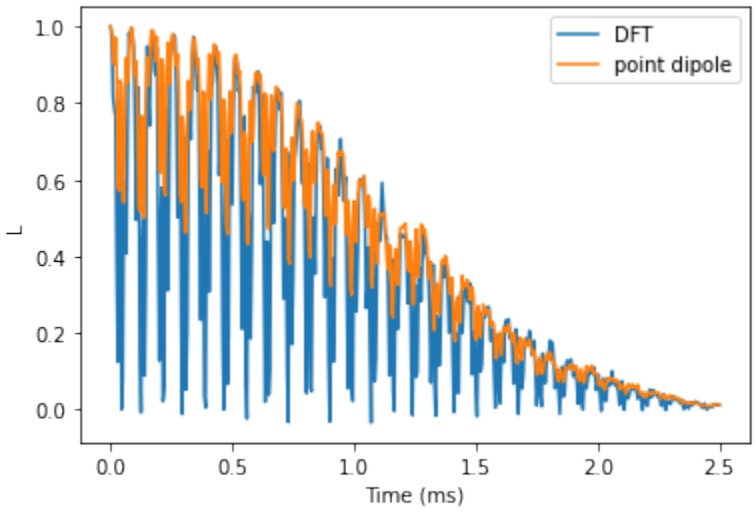
Hahn-echo comparison

Now we compare the predictions for Hahn-echo signal with different hyperfine couplings.

```
he_time = np.linspace(0, 2.5, 501)
B = np.array([0, 0, 500])
N = 1

he_ldft = calc.compute(he_time, magnetic_field=B, pulses=N, as_delay=False)
he_lpd = pdcalc.compute(he_time, magnetic_field=B, pulses=N, as_delay=False)
```

Plot the results and compare. We observe that electron spin echo modulations differ significantly, while the observed decay is about the same.

```
plt.plot(he_time, he_ldft.real, label='DFT')
plt.plot(he_time, he_lpd.real, label='point dipole')

plt.legend()
plt.xlabel('Time (ms)')
plt.ylabel('L');
```



3.2.2 Basal kh-VV in SiC

The basal divacancy's Hamiltonian includes both D and E terms, which allows for mixing between +1 and -1 spin levels at zero field.

Thus, either the generalized CCE should be used, or additional perturbational Hamiltonian terms are to be added. Here we consider the generalized CCE framework.

First, prepare rotation matrix for DFT results. The same supercell was used to compute hyperfine couplings, however z-axis of the electron spin qubit is aligned with Si-C bond, therefore we will need to rotate the DFT supercell accordingly.

```
# Coordinates of vacancies in cell coordinates (note that Vsi is not located in the␣
↪first unitcell)
vsi_cell = -np.array([1 / 3, 2 / 3, 0.0620])
vc_cell = np.array([0, 0, 0])

sic.zdir = [0, 0, 1]

# Rotation matrix for DFT supercell
R = pc.rotmatrix([0, 0, 1], sic.to_cartesian(vsi_cell - vc_cell))
```

Total spin bath can be initiallized by simply setting z direction of the `BathCell` object.

```
sic.zdir = vsi_cell - vc_cell

# Generate bath spin positions
sic.add_isotopes(('29Si', 0.047), ('13C', 0.011))
atoms = sic.gen_supercell(200, remove=[('Si', vsi_cell),
                                       ('C', vc_cell)],
                          seed=seed)
```

Read DFT results with `read_qe` function. To rotate in the correct frame we need to apply both changes of basis consequently

```
M = np.array([[0, 0, -1],
              [0, -1, 0],
              [-1, 0, 0]])

# Position of (0,0,0) point in cell coordinates
center = np.array([0.59401, 0.50000, 0.50000])

# Read GIPAW results
exatoms = pc.read_qe('basal/pw.in',
                     hyperfine='basal/gipaw.out',
                     center=center, rotation_matrix=(M.T @ R),
                     rm_style='col',
                     isotopes={'C':'13C', 'Si':'29Si'})
```

To check whether our rotations produced correct results we can find the indexes of the `BathArray` and DFT output with `pc.same_bath_indexes` function. It returns a tuple, containing the indexes of elements in the two `BathArray` instances with the same position and name. First element of the tuple - indexes of first argument, second - of the second. For that we generate supecell with `BathCell` class, containing 100% isotopes, and count the number of found indexes - iut should be equal to the size of DFT supercell.

```
# isotopes
sic.add_isotopes(('29Si', 1), ('13C', 1))
allcell = sic.gen_supercell(50, remove=[('Si', vsi_cell),
                                        ('C', vc_cell)],
                            seed=seed)

indexes, ext_indexes = pc.same_bath_indexes(allcell, exatoms, 0.2, True)
print(f"There are {indexes.size} same elements."
      f" Size of the DFT supercell is {exatoms.size}")
```

```
There are 1438 same elements. Size of the DFT supercell is 1438
```

Setting up calculations

Now we can safely setup calculations of coherence function with DFT couplings. We will compare results with or without bath state sampling.

```
D = 1.334 * 1e6
E = 0.0184 * 1e6
magnetic_field = 0

calc = pc.Simulator(1, pos, bath=atoms, external_bath=exatoms, D=D, E=E,
                    magnetic_field=magnetic_field, alpha=0, beta=1,
                    r_bath=r_bath, order=CCE_order, r_dipole=r_dipole)
```

The code automatically picks up the two lowest eigenstates of the central spin hamiltonian as qubit states.

```
print(calc)
```

```
Simulator for center array of size 1.
magnetic field:
array([0., 0., 0.])
```

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```
Parameters of cluster expansion:
r_bath: 40
r_dipole: 8
order: 2

Bath consists of 761 spins.

Clusters include:
761  clusters of order 1.
1870  clusters of order 2.
```

We can use the CenterArray, stored in `Simulator.center` attribute, to take a look at the qubit states in the absence of nuclear spin bath.

```
calc.center.generate_states()
print(f'0 state: {calc.alpha.real}; 1 state: {calc.beta.real}')
```

```
0 state: [ 0. -1.  0.]; 1 state: [ 0.70711  0.      -0.70711]
```

Free Induction Decay (FID)

Now, use the generalized CCE to compute FID of the coherence function at different CCE orders.

```
N = 0 # Number of pulses
time_space = np.linspace(0, 1, 101) # Time points at which to compute

orders = [1, 2, 3]
lgen = []

r_bath = 30
r_dipole = 8

calc = pc.Simulator(1, pos, bath=atoms, external_bath=exatoms,
                    D=D, E=E, pulses=N, alpha=0, beta=1,
                    r_bath=r_bath, r_dipole=r_dipole)
```

```
for o in orders:
    calc.generate_clusters(o)
    l = calc.compute(time_space, method='gcce',
                     quantity='coherence', as_delay=False)

    lgen.append(np.abs(l))

lgen = pd.DataFrame(lgen, columns=time_space, index=orders).T
```

We see that the results do not converge, but rather start to diverge. Bath sampling (setting `nbstates` to some value) will help with that.

```
lgen.plot()
plt.xlabel('Time (ms)')
```

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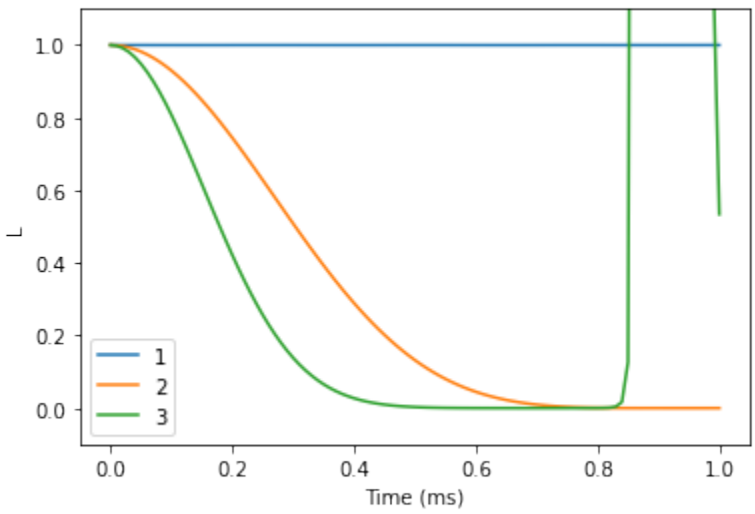
```
plt.ylabel('L')
plt.ylim(-0.1, 1.1);
```



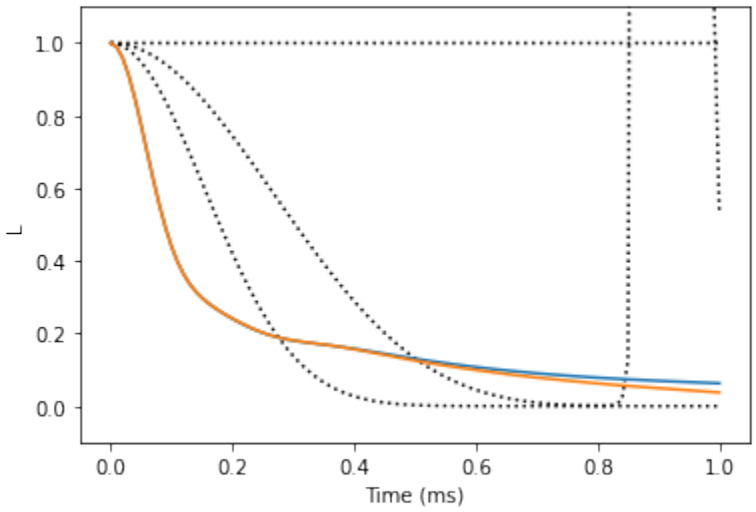
Note, that this approach is `nbstates` times more expensive than the gCCE, therefore the following calculation will take a couple of minutes.

```
orders = [1, 2]
lgcce = []

r_bath = 30
r_dipole = 6

for o in orders:
    calc.generate_clusters(o)

    l = calc.compute(time_space, nbstates=30, seed=seed,
                     method='gcce',
                     quantity='coherence', as_delay=False)

    lgcce.append(np.abs(l))

lgcce = pd.DataFrame(lgcce, columns=time_space, index=orders).T
```

Compare the two results

The gCCE results are converged at 1st order. Note that we used only a small number of bath states (30), thus the calculations are not converged with respect to the number of bath states. Calculations with higher number of bath states (~100) will produce correct results.

```
plt.plot(lgen, color='black', ls=':')
plt.plot(lgcce)

plt.xlabel('Time (ms)')
plt.ylabel('L')
plt.ylim(-0.1, 1.1);
```



Hahn-echo decay

Using the similar procedure to the one used for FID, we can compute the Hahn-echo decay.

```
r_bath = 40
r_dipole = 8
order = 2
N = 1 # Number of pulses

calc = pc.Simulator(1, pos, bath=atoms, external_bath=exatoms,
                    pulses=N, D=D, E=E, alpha=-1, beta=0,
                    r_bath=r_bath, order=order, r_dipole=r_dipole)
```

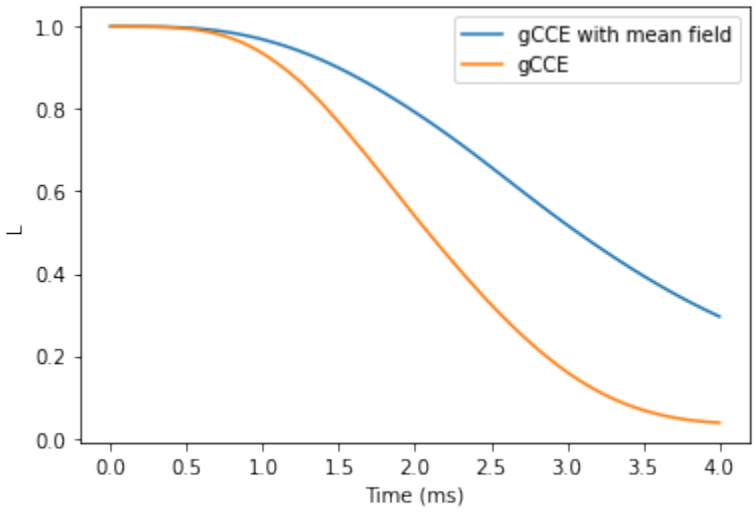
```
ts = np.linspace(0, 4, 101) # time points (in ms)
```

```
helgen = calc.compute(ts, method='gcce', quantity='coherence')
```

Note the number of nbstates leads to significantly increased time of the calculation. The interface to mpi implementation is provided with keywords `parallel` (general) or `parallel_states`(bath state sampling run-specific). However it requires `mpi4py` installed and a run on several cores.

```
helgcce = calc.compute(time_space, nbstates=30, seed=seed,
                       method='gcce', quantity='coherence')
```

```
plt.plot(ts, helgcce, label='gCCE with mean field')
plt.plot(ts, helgen, label='gCCE')

plt.legend()
plt.xlabel('Time (ms)')
plt.ylabel('L');
```



3.3 Shallow donor in Si

Example of more complicated simulations, in which we compare the coherence predicted with point-dipole hyperfine couplings and one obtained using the hyperfines from model wavefunction of the shallow donor in Si (P:Si).

```
import numpy as np
import matplotlib.pyplot as plt
import sys
import ase

import pycce as pc

seed = 8800
np.set_printoptions(suppress=True, precision=5)
```

First, as always, generate spin bath with `BathCell` instance. To get parameters we use ase interface. It allows to conveniently read structure files of any type.

```
# Generate unitcell from ase
from ase import io
s = io.read('si.cif')
s = pc.bath.BathCell.from_ase(s)
# Add types of isotopes
s.add_isotopes(('29Si', 0.047))
# set z direction of the defect
s.zdir = [1, 1, 1]
# Generate supercell
atoms = s.gen_supercell(200, remove=[('Si', [0., 0., 0.])], seed=seed)
```

3.3.1 Calculations with point dipole hyperfine couplings

Here we compute Hahn-echo decay with point dipole hyperfine couplings. All of the parameters are converged, however it never hurts to check!

```
# Parameters of CCE calculations engine

# Order of CCE aproximation
CCE_order = 2
# Bath cutoff radius
r_bath = 80  # in A
# Cluster cutoff radius
r_dipole = 10  # in A

# position of central spin
position = [0, 0, 0]
# Qubit levels (in Sz basis)
alpha = [0, 1]; beta = [1, 0]
# Mag. Field (Bx By Bz)
B = np.array([0, 0, 1000])  # in G
# Number of pulses in CPMG seq (0 = FID, 1 = HE etc)
pulses = 1

# Setting the runner engine
calc = pc.Simulator(spin=0.5, position=position, alpha=alpha, beta=beta,
                    bath=atoms, r_bath=r_bath, magnetic_field=B, pulses=pulses,
                    r_dipole=r_dipole, order=CCE_order)
```

```
# Time points
time_space = np.linspace(0, 2, 201)  # in ms
```

For comparison, we compute both with generalized CCE and usual CCE coherence. Note a relatively large bath (`r_bath = 80`), so the calculations will take some time.

```
l_cce = calc.compute(time_space, method='CCE')
l_gen = calc.compute(time_space, method='gCCE')
```

3.3.2 Hyperfine couplings of the shallow donor

We compute the hyperfine couplings of the shallow donnor, following the formulae by Rogerio de Sousa and S. Das Sarma (Phys Rev B 68, 115322 (2003)).

```
# PHYSICAL REVIEW B 68, 115322 (2003)
n = 0.81
a = 25.09

def factor(x, y, z, n=0.81, a=25.09, b=14.43):
    top = np.exp(-np.sqrt(x**2/(n*b)**2 + (y**2 + z**2)/(n*a)**2))
    bottom = np.sqrt(np.pi * (n * a)**2 * (n * b) )

    return top / bottom
```

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```
def contact_si(r, gamma_n, gamma_e=pc.ELECTRON_GYRO, a_lattice=5.43, nu=186, n=0.81,␣
↪a=25.09, b=14.43):
    k0 = 0.85 * 2 * np.pi / a_lattice
    pre = 8 / 9 * gamma_n * gamma_e * pc.HBAR_MU0_O4PI * nu
    xpart = factor(r[0], r[1], r[2], n=n, a=a, b=b) * np.cos(k0 * r[0])
    ypart = factor(r[1], r[2], r[0], n=n, a=a, b=b) * np.cos(k0 * r[1])
    zpart = factor(r[2], r[0], r[1], n=n, a=a, b=b) * np.cos(k0 * r[2])
    return pre * (xpart + ypart + zpart) ** 2
```

We make a copy of the `BathArray` object, and set up their hyperfines according to the reference above.

```
newatoms = atoms.copy()

# Generate hyperfine from point dipole
newatoms.from_point_dipole(position)

# Following PRB paper
newatoms['A'][newatoms.dist() < n*a] = 0
newatoms['A'] += np.eye(3)[np.newaxis,:,:] * contact_si(newatoms['xyz'].T, newatoms.
↪types['29Si'].gyro)[:,np.newaxis, np.newaxis]
```

Now we set up a `Simulator` object. Because hyperfines in `newatoms` are nonzero, they are **not** approximated as the ones of point dipole.

```
calc = pc.Simulator(spin=0.5, position=position, alpha=alpha, beta=beta,
                    bath=newatoms, r_bath=r_bath, magnetic_field=B, pulses=pulses,
                    r_dipole=r_dipole, order=CCE_order)
```

```
shallow_l_cce = calc.compute(time_space, method='CCE')
shallow_l_gen = calc.compute(time_space, method='gCCE')
```

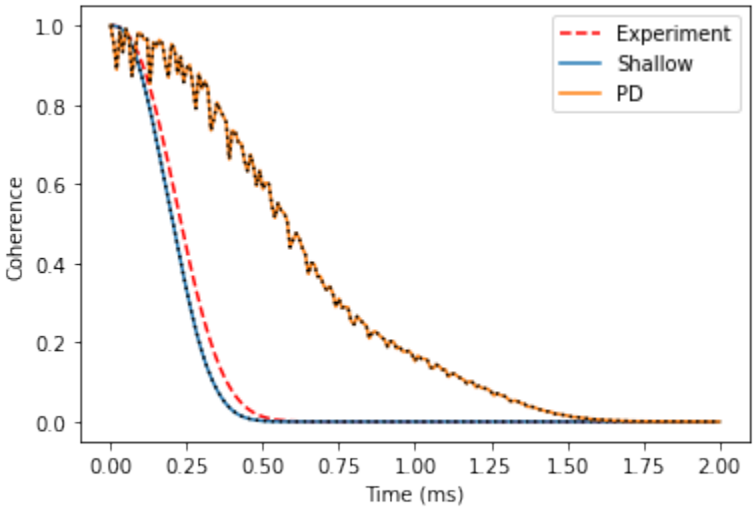
3.3.3 Compare the results

We find that the point dipole gives a poor agreement with the experimental data. Model wavefunction, on the countrary, produces great agreement with the experimental coherence time from work of Eisuke Abe et al. (Phys Rev B 82, 121201(R) (2010)).

```
t2exp = 0.27 # Experimental T2 from PhysRevB.82.121201
decay = lambda t: np.exp(-(t/t2exp)**2.4)
plt.plot(time_space, decay(time_space), color='red', label='Experiment', ls='--')

plt.plot(time_space, shallow_l_cce.real, label='Shallow')
plt.plot(time_space, shallow_l_gen.real, ls=':', c='black')

plt.plot(time_space, l_cce.real, label='PD')
plt.plot(time_space, l_gen.real, ls=':', c='black')
plt.legend();
plt.xlabel('Time (ms)')
plt.ylabel('Coherence');
```



Interesting to note - the decay depends significantly on the orientation of the magnetic field. You can check it yourself!

3.4 Correlation function

In this tutorial we will compute the coherence function of the NV Center in diamond and then reproduce it from the correlation function of the noise.

The correlation function $C(t)$ of the effective magnetic field (noise) along the z-axis can be defined as follows:

$$C(t) = \langle \beta_z(t) \beta_z(0) \rangle \tag{3.1}$$

With β_z given as:

$$\beta_z(t) = U^\dagger(t) \left(\sum_{\{I\}} A_{zz} I_z \right) U(t) \tag{3.2}$$

Where $U(t)$ is time propagator.

Within the CCE formalism, the correlation function is computed as:

$$C(t) = \sum_{\{i\}} \tilde{C}_{\{i\}}(t) + \sum_{\{ij\}} \tilde{C}_{\{ij\}}(t) \; + \; ... \tag{3.3}$$

With contributions computed as:

$$\tilde{C}_\nu(t) = C_\nu(t) - \sum_{\nu' \subset \nu} \tilde{C}_{\nu'}(t) \tag{3.4}$$

```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
```

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```
import sys

import pycce as pc
import ase

seed = 42055
np.set_printoptions(suppress=True, precision=5)
```

3.4.1 Generate nuclear spin bath

Building a `BathArray` of nuclear spins from the `ase.Atoms` object.

```
from ase.build import bulk

# Generate unitcell from ase
diamond = bulk('C', 'diamond', cubic=True)
diamond = pc.bath.BathCell.from_ase(diamond)
# Add types of isotopes
diamond.add_isotopes(('13C', 0.011))
# set z direction of the defect
diamond.zdir = [1, 1, 1]
# Add the defect. remove and add atoms at the positions (in cell coordinates)
atoms = diamond.gen_supercell(200, remove=[('C', [0., 0, 0]),
                                           ('C', [0.5, 0.5, 0.5])],
                              add=('14N', [0.5, 0.5, 0.5]),
                              seed=seed)
```

Next, we define all of the parameters of the simulation. We are interested in the very specific regime, when all nearby nuclear spins are removed. To achieve this goal we define an `inner = 20` parameter, and remove all nuclear spins within this radius.

```
position = np.array([0, 0, 0])
inner = 20
smallatoms = atoms[atoms.dist(position) >= inner]

parameters = dict(
    order=2, # CCE order
    r_bath=60,  # Size of the bath in A
    r_dipole=6,  # Cutoff of pairwise clusters in A
    position=position, # Position of central Spin
    alpha=[0, 0, 1], # 0 qubit state
    beta=[0, 1, 0], # 1 qubit state
    magnetic_field = 500, # magnetic field along z-axis
    pulses=1 # N pulses in CPMG sequence
) # Qubit levels

ts = np.linspace(0, 2.5, 1001)  # Time points in ms
```

3.4.2 Coherence calculations

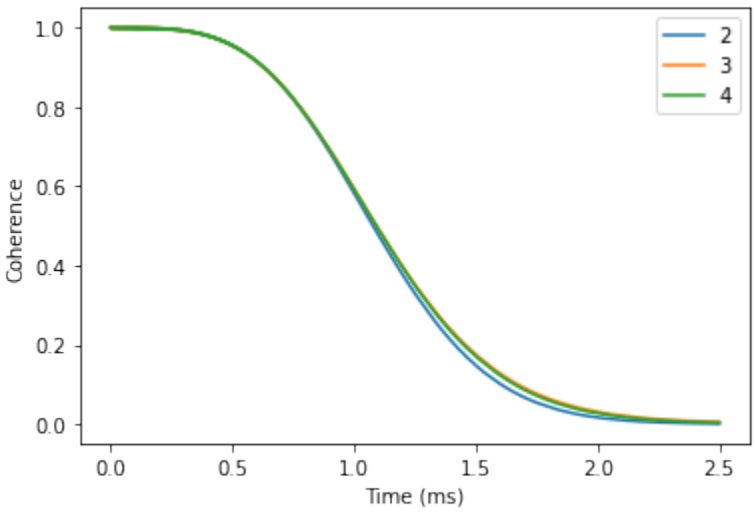
Next, we set up `Simulator` objects and check convergence with respect to the CCE order.

```
calc = pc.Simulator(spin=1, bath=smallatoms, **parameters)
```

```
orders = [2, 3, 4]
coh = {}
for o in orders:
    calc.generate_clusters(o)
    coh[o] = calc.compute(ts, method='cce', quantity='coherence')
coh = np.abs(pd.DataFrame(coh, index=ts))
coh.index.name = 'Time (ms)'
```

Visually verify the convergence.

```
coh.plot()
plt.ylabel('Coherence');
```

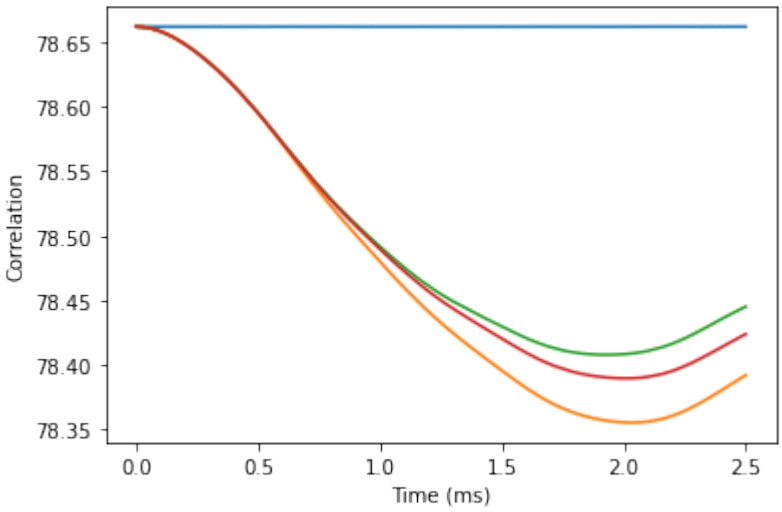


3.4.3 Noise calculations

To compute the correlation function of the noise, we call `Simulator.compute` method and specify `quantity = 'noise'`.

First we determine convergence of the correlation function with the CCE order.

```
for o in [1, 2, 3, 4]:
    calc.generate_clusters(o)
    noise = calc.compute(ts, method='cce', quantity='noise')
    plt.plot(ts, noise.real, label=o)
plt.xlabel('Time (ms)')
plt.ylabel('Correlation');
```



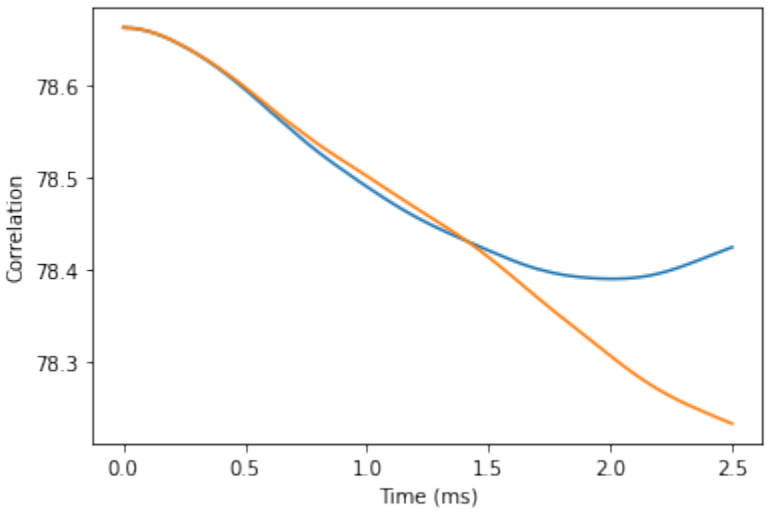
The difference between third and fourth order is fairly small, we will use the fourth order for the following calculations. It will take a bit of a time, so you can grab some tea while you wait.

```
calc.generate_clusters(4)

noise = calc.compute(ts, method='cce', quantity='noise')
genoise = calc.compute(ts, method='gcce', quantity='noise', nbstates=0)
```

Compare the results obtained with CCE and gCCE approaches. Note that they are slighlity different. However, as we will see it does not impact the predicted coherence.

```
plt.plot(ts, noise.real, label='CCE')
plt.plot(ts, genoise.real, label='gCCE')
plt.xlabel('Time (ms)')
plt.ylabel('Correlation');
```



Assuming that the noise is Gaussian, we can reproduce the coherence from the average phase squared $\langle\phi^2\rangle$, accumulated by the spin qubit:

$L(t) = e^{-\langle\phi^2(t)\rangle}$

The average phase is obtained from the autocorrelation function as:

$\langle\phi^2(t)\rangle = \int_0^t d\tau C(\tau)F(\tau)$

Where $F(\tau)$ is the correlation filter function (see Phys. Rev. A 86, 012314 (2012) for details).

PyCCE code already has implemented calculations of the phase in the `pycce.filter` module:

`pycce.filter.gaussian_phase` takes three positional arguments: - `timespace` - time points at which correlation function was computed; - `corr` - noise autocorrelation function; - `npulses` - number of pulses in CPMG sequence.

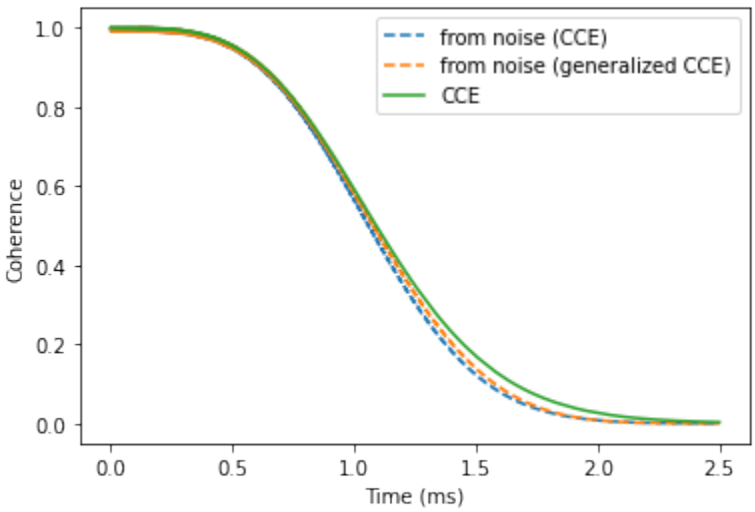
Here we compute the phase for the Hahn-echo experiment. Note that the implementation of `gaussian_phase` is not heavily optimized and can take a hot second.

```
import pycce.filter

chis =  pycce.filter.gaussian_phase(ts, np.abs(noise), 1)
gchis = pycce.filter.gaussian_phase(ts, np.abs(genoise), 1)
```

Now compare results from direct calculations of the coherence function, and the one reconstructed from the noise autocorrelation:

```
plt.plot(ts, np.exp(-chis).real, ls='--', label='from noise (CCE)')
plt.plot(ts, np.exp(-gchis).real, ls='--', marker='', label='from noise (generalized CCE)
↪')
plt.plot(ts, coh[4], label='CCE')
plt.legend()
plt.xlabel('Time (ms)')
plt.ylabel('Coherence');
```



3.5 Multiple central spins

Instead of one central spin, the PyCCE can be used to consider the dynamics of N central spins.

Then the central spin Hamiltonian and spin-bath Hamiltonian are written as:

$$\hat{H}_S = \sum_i \mathbf{S_i D_i S_i} + \mathbf{S_i} \gamma_{\mathbf{S_i}} \mathbf{B} + \sum_{i<j} \mathbf{S_i K_{ij} S_j} \tag{3.5}$$

Where $\mathbf{K_{ij}}$ are interaction tensors between central spins i and j.

The central spin-bath couplings can be defined as:

$$\hat{H}_{SB} = \sum_{i,l} \mathbf{S_i A_{il} I_l} \tag{3.6}$$

```
!pip install pycce
!pip install ase

import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

import sys
import pycce as pc
import ase

seed = 8805
np.random.seed(seed)
np.set_printoptions(suppress=True, precision=4)
```

3.5.1 Two NV Centers in Diamond

First example is two NV centers in diamond. We begin by considering two non-interacting electron spins in the nuclear spin bath.

We generate the nuclear ^{13}C spin bath using a well-defined procedure.

```
from ase.build import bulk

# Generate unitcell from ase
diamond = pc.read_ase(bulk('C', 'diamond', cubic=True))
diamond.zdir = [1,1,1]

bath = diamond.gen_supercell(200, seed=seed, remove=('C', [0,0,0]))
```

Generating the CenterArray object

The properties of the NVs are stored in the CenterArray.

CenterArray object contains the properties of all central spins in the system. In this example, we prepare the array consisting of two electron spin-1, with the same ZFS and gyromagnetic ratio.

```
D = 2.4e6  # in kHz
gyro = pc.ci['e'].gyro  # gyromagnetic ratio of electron in rad/G/ms

# Generate an array of two central spins,
# each with the same D and gyromagnetic ratio value,
# separated by 100 nm.
nvs = pc.CenterArray(spin=[1, 1], D=[D, D],
                     position=[[0, 0, 0], [0, 0, 1000]],
                     gyro=[gyro, gyro], alpha=0, beta=2)

print(nvs)  # Print properties of the central spin array
```

```
CenterArray
(s: [1. 1.],
xyz:
[[   0.    0.    0.]
 [   0.    0. 1000.]],
zfs:
[[[-800000.       0.       0.]
  [      0. -800000.       0.]
  [      0.       0. 1600000.]]

 [[-800000.       0.       0.]
  [      0. -800000.       0.]
  [      0.       0. 1600000.]]],
gyro:
[[[-17608.5971     -0.         -0.    ]
  [    -0.     -17608.5971     -0.    ]
  [    -0.         -0.     -17608.5971]]

 [[-17608.5971     -0.         -0.    ]
  [    -0.     -17608.5971     -0.    ]
  [    -0.         -0.     -17608.5971]]])
```

You can access the properties of the central spins (and modify them) as items in CenterArray.

```
print(nvs[0], '\n')
nvs[0].gyro = np.random.random((3,3)) * 1000
print(nvs)
nvs[0].gyro = np.eye(3) * pc.ELECTRON_GYRO
```

```
Center
(s: 1.0,
xyz:
[0. 0. 0.],
zfs:
[[-800000.       0.       0.]
 [      0. -800000.       0.]
```

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```
 [      0.       0. 1600000.]],
gyro:
-17608.59705)

CenterArray
(s: [1. 1.],
xyz:
[[   0.    0.    0.]
 [   0.    0. 1000.]],
zfs:
[[[-800000.       0.       0.]
  [      0. -800000.       0.]
  [      0.       0. 1600000.]]

 [[-800000.       0.       0.]
  [      0. -800000.       0.]
  [      0.       0. 1600000.]]],
gyro:
[[[   989.9394    629.7526    554.6254]
  [   641.9013    943.0174     56.2197]
  [   568.4803    978.1593    265.0863]]

 [[-17608.5971     -0.         -0.    ]
  [    -0.     -17608.5971     -0.    ]
  [    -0.         -0.     -17608.5971]]])
```

For illustrative purposes, we will use identical nuclear spin environment for two NVs. For that we create a copy of the `BathArray`, shift it by 1000 angstroms, and concatenate two arrays.

The `CenterArray` instance is provided as a `spin` keyword to the `Simulator` object. It can be later accesed as `Simulator.center` attribute.

```
bath2 = bath.copy()
bath2.z += 1000

calc = pc.Simulator(spin=nvs, bath=np.concatenate([bath, bath2]),
                    r_bath=[40, 40], r_dipole=6, order=2, magnetic_field=500)
print(calc)
```

```
Simulator for center array of size 2.
magnetic field:
array([  0.,   0., 500.])

Parameters of cluster expansion:
r_bath: [40, 40]
r_dipole: 6
order: 2

Bath consists of 1046 spins.

Clusters include:
1046  clusters of order 1.
836  clusters of order 2.
```

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When the number of central spins is greater than one, hyperfine couplings in the `BathArray` have an additional dimension, corresponding to the two sets of the hyperfine couplings.

```
print(calc.bath.A.shape)
print(calc.bath[0].A)
```

```
(1046, 2, 3, 3)
[[[ 2.3048  1.1078 -0.6608]
  [ 1.1078 -1.0451 -0.1988]
  [-0.6608 -0.1988 -1.2597]]

 [[-0.      0.      0.    ]
  [ 0.     -0.      0.    ]
  [ 0.      0.      0.    ]]]
```

Decoherence of entangled state

Let's do some calculations! Note that `gcce` method in this case includes a lot (9-fold) larger Hilbert space, so it will take a bit longer.

Here we compute the coherence function, defined as a decay of the offdiagonal element of the density matrix:

$$L = \langle 0|\hat{\rho}|1\rangle \tag{3.7}$$

Where $|0\rangle$ and $|1\rangle$ are defined as eigenstates of the central spin Hamiltonian introduced above.

```
ts = np.linspace(0, 2)
calc.alpha = 0 # 00 state
calc.beta = 1 # -10 state
cce = {}
gcce = {}

cce['01'] = calc.compute(ts, pulses=1)
gcce['01'] = calc.compute(ts, method='gcce', pulses=1)

calc.beta = 1 # 0-1 state
cce['02'] = calc.compute(ts, pulses=1)
gcce['02'] = calc.compute(ts, method='gcce', pulses=1)

calc.beta = 3 # -1 -1 state
%time cce['03'] = calc.compute(ts, pulses=1)
%time gcce['03'] = calc.compute(ts, method='gcce', pulses=1)
```

```
/home/onizhuk/midway/codes_development/pyCCE/pycce/h/functions.py:298:␣
↪NumbaPerformanceWarning: '@' is faster on contiguous arrays, called on␣
↪(array(complex128, 2d, A), array(complex128, 2d, A))
  hself = vec_tensor_vec(svec, tensor, svec)
/home/onizhuk/midway/codes_development/pyCCE/pycce/h/functions.py:298:␣
↪NumbaPerformanceWarning: '@' is faster on contiguous arrays, called on␣
```

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```
↪(array(complex128, 2d, A), array(complex128, 2d, A))
  hself = vec_tensor_vec(svec, tensor, svec)
```

```
CPU times: user 1.72 s, sys: 20.3 ms, total: 1.74 s
Wall time: 629 ms
CPU times: user 2min 22s, sys: 1.99 s, total: 2min 24s
Wall time: 24.4 s
```

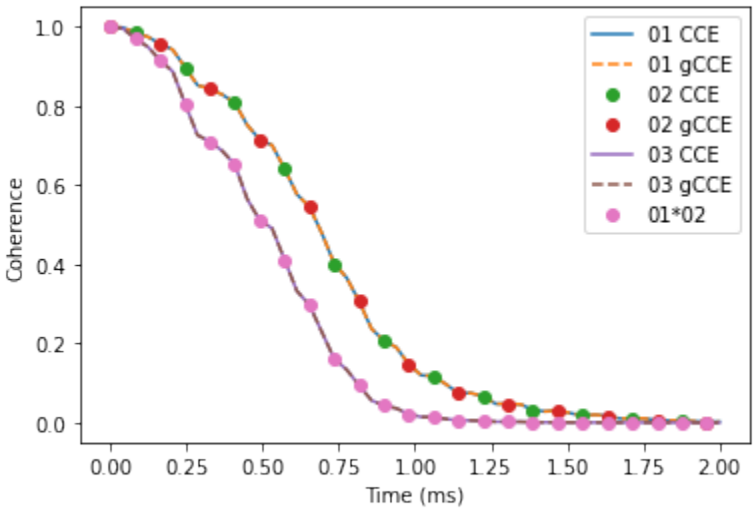
As expected, in the case of decoupled NV centers the coherence of the bell state decays as a product of separated NVs decoherence.

```
plt.plot(ts, cce['01'].real, label='01 CCE')
plt.plot(ts, gcce['01'].real, ls='--', label='01 gCCE')

plt.plot(ts, cce['02'].real, markevery=(2, 4), ls='', marker='o', label='02 CCE')
plt.plot(ts, gcce['02'].real, ls='', marker='o', markevery=4, label='02 gCCE')

plt.plot(ts, cce['03'].real, label='03 CCE')
plt.plot(ts, gcce['03'].real, ls='--', label='03 gCCE')

plt.plot(ts, gcce['02'].real * gcce['01'].real, ls='', marker='o', markevery=2, label=
↪'01*02')
plt.ylabel('Coherence')
plt.xlabel('Time (ms)')
plt.legend();
```



Entanglement between two NVs

We can use the PyCCE to predict how the entanglement evolves between two dipolarly coupled electron spins, initially prepared in the product state:

$$|\Psi\rangle = \frac{1}{2}(|0\rangle + |-1\rangle) \otimes (|0\rangle + |-1\rangle) \tag{3.8}$$

We add interaction between two NVs by calling `nvs.point_dipole` method, that generates interaction tensors from point dipole approximation. We can also directly set interaction tensors by calling `nvs.add_interaction` method or modifiying `nvs.imap` attribute.

```
nvs = pc.CenterArray(spin=[1, 1], D=[D, D],
                     position=[[0, 0, 0], [0, 0, 50]],
                     gyro=[gyro, gyro], alpha=0, beta=2)

nvs.point_dipole() # Add interactions

zero = np.array([0, 1, 0])
one  = np.array([0, 0, 1])
nvs[0].alpha = zero # Set qubit levels
nvs[0].beta = one
nvs[1].alpha = one
nvs[1].beta = zero

# Generate product state
state = pc.normalize(np.kron(zero + one, zero + one))
nvs.state = state
print("Initial amplitudes in Sz x Sz basis:", np.abs(nvs.state)) # Initial state
print("Interaction tensor:")
print(nvs.imap[0, 1]) # in kHz
```

```
Initial amplitudes in Sz x Sz basis: [0.  0.  0.  0.  0.5 0.5 0.  0.5 0.5]
Interaction tensor:
[[ 416.3281   -0.       -0.    ]
 [  -0.      416.3281   -0.    ]
 [  -0.       -0.     -832.6562]]
```

We will use negativity (https://en.wikipedia.org/wiki/Negativity_(quantum_mechanics)) as a metric of entanglement, defined as:

$ N‘(:nbsphinx-math:rho`) ≡ ‘ : $nbsphinx - math : frac{||rhoˆ{Gamma_A}||_1 - 1}{2}‘$

```
#          0      1     2     3      4     5     6       7       8
states = ['11', '10', '1-1', '01', '00', '0-1', '-11', '-10', '-1-1']

def pltdm(t, dm, ax):
    """
    Function to plot nonzero elements of the density matrix.
    """
    for i, j in np.argwhere(np.triu(dm[0])):
        label=r'$\langle$' + f'{states[i]}'+r'$|\rho|$'+ f'{states[j]}'+ r'$\rangle$'
        ax.plot(t, np.abs(dm[:, i, j]), label=label)
```

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```
def partial_transpose(dm0, dim, which):
    """
    Get partial transpose of the density matrix.
    """
    ish = dm0.shape
    n = len(dim)
    indexes = np.arange(len(dim)*2)
    indexes[which] = n + which
    indexes[n + which] = which
    return dm0.reshape(*dim, *dim).transpose(*indexes).reshape(ish)

def negativities(dms):
    """
    Compute negativity for an array of density matrices.
    """
    negs = []
    for dm in dms:
        pt = partial_transpose(dm, [3,3], 0)
        tr_norm = np.linalg.norm(pt, ord='nuc')
        negs.append((tr_norm - 1) / 2)
    return np.array(negs)

def rz(dm):
    """
    Set density matrix elements equal to zero at zero timepoint to zero.
    Removes numerical instabilities when we divide by a near-zero value.
    """
    dm[np.broadcast_to((dm[0] == 0), dm.shape)] = 0
    return dm
```

First, compute the entanglement without dynamical decoupling pulses applied.

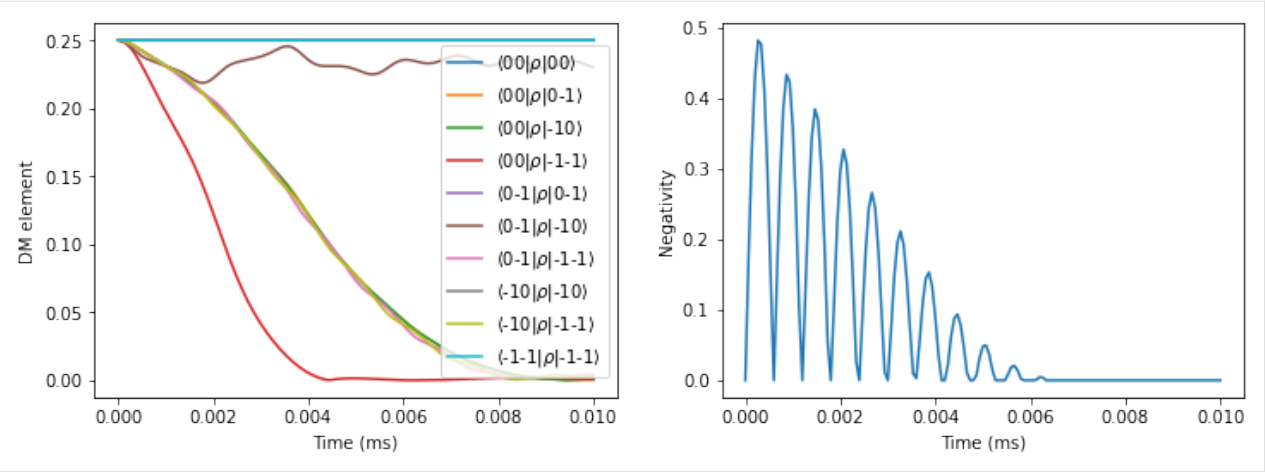
```
tfid = np.linspace(0, 0.01, 151)

c = pc.Simulator(nvs, bath=bath, r_bath=40, r_dipole=6,
                 order=2, pulses=0, magnetic_field=500)
dmfid = rz(c.compute(tfid, method='gcce', fulldm=True))
```

```
fig, axes = plt.subplots(1, 2, figsize=(12, 4))

pltdm(tfid, dmfid, axes[0])
axes[1].plot(tfid, negativities(dmfid))

axes[0].legend()
axes[0].set(ylabel='DM element', xlabel='Time (ms)')
axes[1].set(ylabel='Negativity', xlabel='Time (ms)');
```



Compare that to the case, when π pulse is applied to each of the electron spins.

To create such pulse sequence, we specify the `which` keyword argument of the `Pulse` class with indexes of both NVs in the `CenterArray`.

```
# Pulse, flipping simultaneously the two NVs
p = pc.Pulse('x', np.pi, which=[0, 1])
the = np.linspace(0, 0.3, 151)

c = pc.Simulator(nvs, bath=bath, r_bath=40, r_dipole=6,
                 order=2, pulses=[p], magnetic_field=500)

dm_short = rz(c.compute(tfid, method='gcce', fulldm=True))
dm = rz(c.compute(the, method='gcce', fulldm=True))
```

As expected, we find a significantly prolonged entanglement between two electron spins.

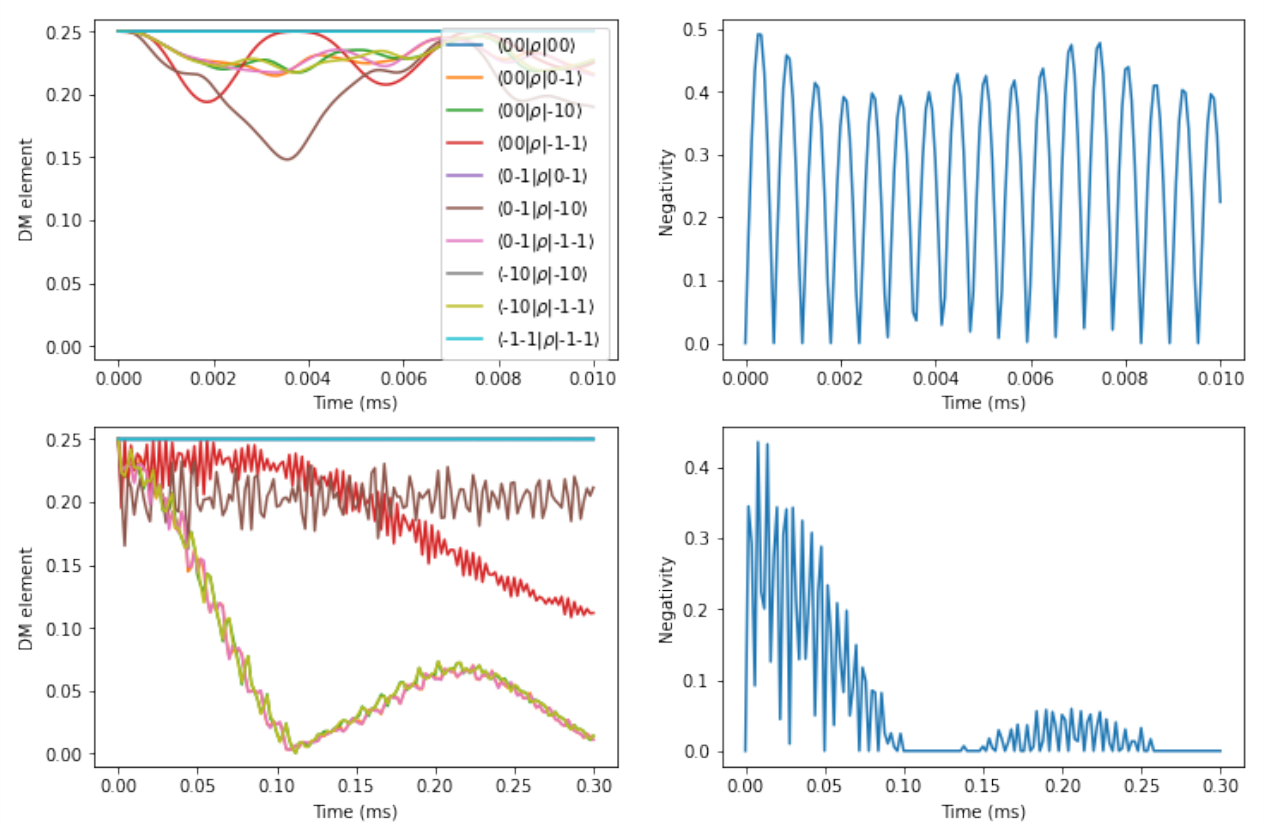
```
fig, axes = plt.subplots(2, 2, figsize=(12, 8))

pltdm(tfid, dm_short, axes[0, 0])
axes[0, 1].plot(tfid, negativities(dm_short))

pltdm(the, dm, axes[1, 0])
axes[1, 1].plot(the, negativities(dm))

axes[0, 0].legend()

for row in axes:
    row[0].set(ylabel='DM element', xlabel='Time (ms)', ylim=(-0.01, 0.26))
    row[1].set(ylabel='Negativity', xlabel='Time (ms)')
```



3.5.2 Si:Bi donor

We use the PyCCE framework to reproduce paper: PHYSICAL REVIEW B 91, 245416 (2015) by S. J. Balian et al. Here, ^{209}Bi nuclear spin 9/2 and electron spin 1/2 interact very strongly (~1.5 GHz hyperfine), with many avoided crossings arising and leading to clock transitions. The qubit states is chosen as a two energy levels of the hybrid electron and nuclear spins system.

First, we prepare a `CenterArray`, containing the properties of two central spins.

```
aiso = 1.4754e6
im = np.eye(3) * aiso # Isotropic interaction tensor
ebi = pc.CenterArray(spin=[1/2, 9/2],
                     gyro=[pc.ci['e'].gyro, pc.ci['209Bi'].gyro],
                     imap=im, alpha=6, beta=13)
```

For visualization purposes, plot a diagram of the energies of the hybrid system as a function of magnetic field. Here the chosen qubit levels are highlighted with black points.

```
ens = []
ms = np.linspace(0, 4000, 51)  # applied magnetic field
for mf in ms:
    ebi.generate_states([0,0, mf])
    ens.append(ebi.energies)

ens = np.asarray(ens)
```

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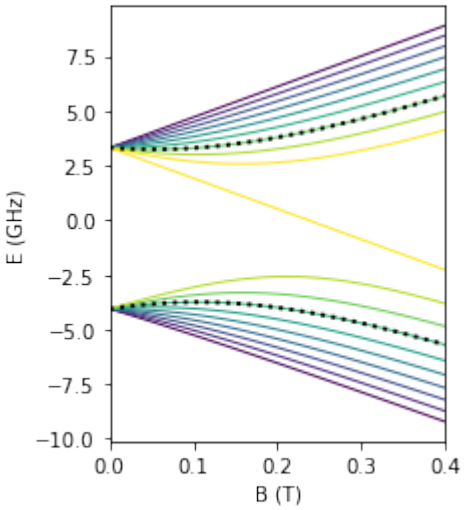
```
lowerdf = pd.DataFrame(ens[:, :10]/1e6, index=ms/1e4,
                       columns=np.arange(10))
higherdf = pd.DataFrame(ens[:, :10:-1]/1e6, index=ms/1e4,
                        columns=np.arange(11, ens.shape[1])[::-1])

fig, ax = plt.subplots(figsize=(3, 4))

lowerdf.plot(ax=ax, cmap='viridis', legend=False, lw=1)
higherdf.plot(ax=ax, cmap='viridis', legend=False, lw=1)
lowerdf[6].plot(ax=ax, color='black', ls=':', lw=2)
higherdf[13].plot(ax=ax, color='black', ls=':', lw=2)
ax.set(xlabel='B (T)', ylabel='E (GHz)', xlim=(0, 0.4));
```



Now we define the calculations of hyperfine couplings for the electron spin.

```
# PHYSICAL REVIEW B 68, 115322 (2003)
#  https://link.springer.com/content/pdf/10.1007%2FBF02725533.pdf for Bi
n_parameter = np.sqrt(0.029/0.069)
# https://journals.aps.org/pr/pdf/10.1103/PhysRev.114.1219
a_parameter = 25.09

def factor(x, y, z, n=n_parameter, a=a_parameter, b=14.43):
    top = np.exp(-np.sqrt(x ** 2 / (n * b) **2 + (y ** 2 + z ** 2) / (n * a) ** 2))
    bottom = np.sqrt(np.pi * (n * a) ** 2 * (n * b) )

    return top / bottom

def contact_si(r, gamma_n, gamma_e=pc.ELECTRON_GYRO,
               a_lattice=5.43, nu=186, n=n_parameter,
               a=a_parameter, b=14.43):

    k0 = 0.85 * 2 * np.pi / a_lattice
    pre = 8 / 9 * gamma_n * gamma_e * pc.HBAR_MU0_O4PI * nu
    xpart = factor(r[0], r[1], r[2], n=n, a=a, b=b) * np.cos(k0 * r[0])
```

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```
    ypart = factor(r[1], r[2], r[0], n=n, a=a, b=b) * np.cos(k0 * r[1])
    zpart = factor(r[2], r[0], r[1], n=n, a=a, b=b) * np.cos(k0 * r[2])
    return pre * (xpart + ypart + zpart) ** 2


def func(bath):
    na = np.newaxis
    aiso = contact_si(bath.xyz.T, bath.gyro) # Contact term
    # Generate dipolar terms
    bath.from_center(ebi)
    # Add contact term for electron spni
    bath.A[:, 0] += np.eye(3)[na, :, :] * aiso[:, na, na]
```

And prepare the spin bath using `ase` interface.

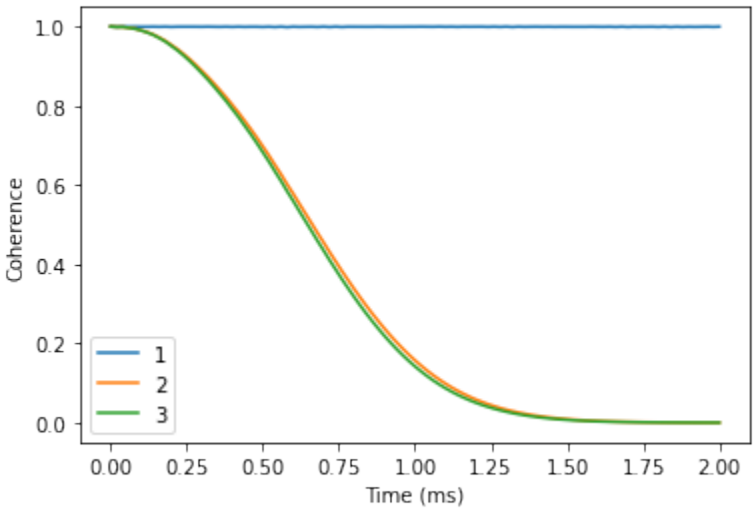
```
si = pc.read_ase(bulk('Si', cubic=True))
atoms = si.gen_supercell(200, remove=('Si', [0., 0, 0]), seed=seed)
```

Away from avoided crossings

Chosen energy levels 6 <-> 14 give raise to the clock transition (CT) at ~800 G. First compute the coherence avay from CT at 3200 G. It will take some time, as the bath is large.

```
nts = np.linspace(0, 2, 101)
sicalc = pc.Simulator(ebi, bath=atoms, r_bath=80, r_dipole=6,
                      order=2, magnetic_field=3200, pulses=1,
                      hyperfine=func)
orders = [1, 2, 3]

ls = []
for v in orders:
    sicalc.order = v
    ls.append(sicalc.compute(nts).real)

dfoff = pd.DataFrame(ls, columns=nts, index=orders).T
```

```
dfoff.plot()
plt.xlabel('Time (ms)')
plt.ylabel('Coherence');
```

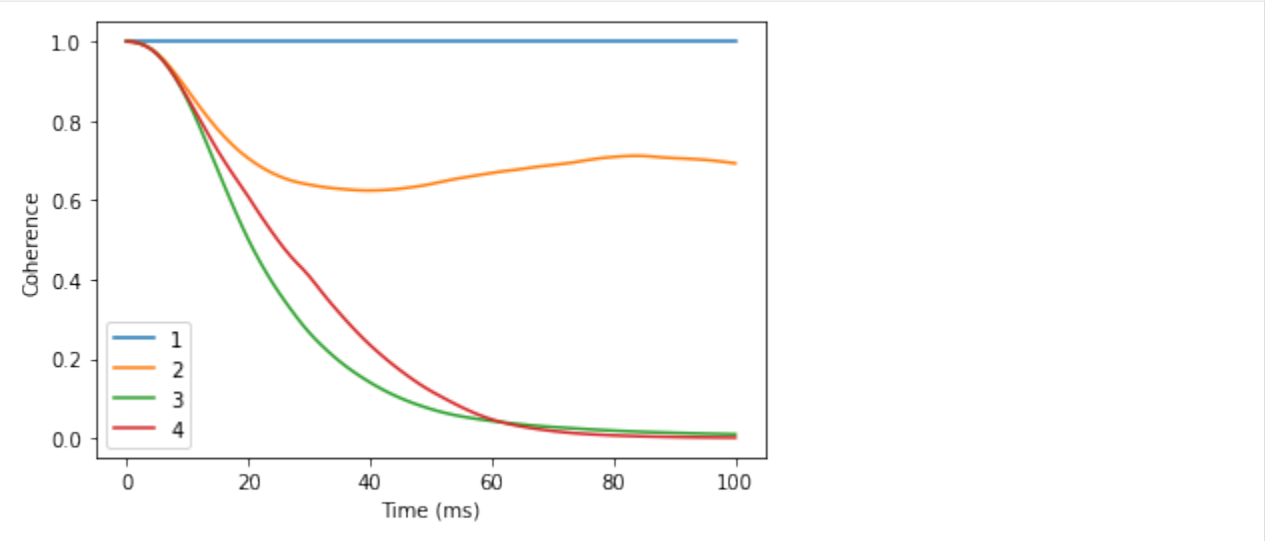


Near avoided crossings

Now compare that to the coherence near the CT (-4G from CT). Note, that number of clusters considered here is already rather large, so the calculations will take a minute or two.

```
ts = np.linspace(0, 100, 101)

sicalc.magnetic_field = 791
orders = [1, 2, 3, 4]

ls = []
for v in orders:
    sicalc.order = v
    ls.append(sicalc.compute(ts).real)

dfat = pd.DataFrame(ls, columns=ts, index=orders).T
```

```
dfat.plot()
plt.xlabel('Time (ms)')
plt.ylabel('Coherence');
```



Exactly at CT one needs even higher `order`, larger `r_bath` and `r_dipole`, and random bath state sampling to get accurate results. It is left as an exersize to the reader to try and converge the coherence at clock transition.

3.6 Dissipative spin bath

In this tutorial we will go over the steps needed to simulate the decoherence of a central spin coupled to a dissipative, interacting spin baths governed by Lindblad Master equation using CCE method (ME-CCE) within the **PyCCE** module. Two methods of interest include:

- Master Equation CCE (ME-CCE).
- Master Equation gCCE (ME-gCCE).

The Lindblad master equation of the overall system can be written as:

:nbsphinx-math:`begin{equation}
frac{d}{dt} hat rho=-frac{i}{hbar}[hat H, hat rho]+sum_i{gamma_i (hat L_i hat rho hat L_i^dagger - frac{1}{2}{hat L_i^dagger hat L_i, hat rho })},

end{equation}`

where $\hat{\rho}$ is the density matrix of the system, $\hat{H}$ is the Hamiltonian, and $\hat{L}_i$ are jump operators with corresponding dissipation rates γ_i.

Within the conventional CCE framework, the coherence of the central spin is recovered from the trace of the partial inner product $\hat{\rho}_{01}(t) = 0\hat{\rho}(t)1$ as $\mathcal{L}(t) = [\hat{\rho}_{01}(t)]/[\hat{\rho}_{01}(0)]$. The evolution of $\hat{\rho}_{01}$ by solving the following:

:nbsphinx-math:`begin{equation}
frac{d}{dt} hat rho_{01} (t) = mathfrak{I} cdot hat rho_{01} (t)= -frac{i}{hbar} hat H^{(0)} hat rho_{01}(t) + frac{i}{hbar} hat rho_{01}(t) hat H^{(1)} + sum_i{gamma_i (hat L_i hat rho hat L_i^dagger - frac{1}{2}{hat L_i^dagger hat L_i, hat rho })},

end{equation}`

Within the generalized CCE framework, one needs to solve full Lindbladian for each cluster including central spin.

```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import pycce as pc
```

3.6.1 Setup the simulator properties

As an example we consider the dissipative electron spin bath. First, we generate electron spin bath with concentration $\rho = 10^{16}$ cm^{-3}

```
electrons = pc.random_bath('e', [5e3, 5e3, 5e3], density=1e16,
                           density_units='cm-3', seed=2)  # Density in 1/cm^3
```

The properties of the central spin-1/2 are stored in the `CenterArray`.

```
center = pc.CenterArray(spin=1/2, alpha=[1,0], beta=[0,1])
print(center)
```

```
CenterArray
(s: [0.5],
xyz:
[[0. 0. 0.]],
zfs:
[[[0. 0. 0.]
  [0. 0. 0.]
  [0. 0. 0.]]],
gyro:
[[[-17608.59705     -0.          -0.      ]
  [    -0.      -17608.59705     -0.      ]
  [    -0.          -0.      -17608.59705]]])
```

To run the simulations we need to setup the `Simulator` object.

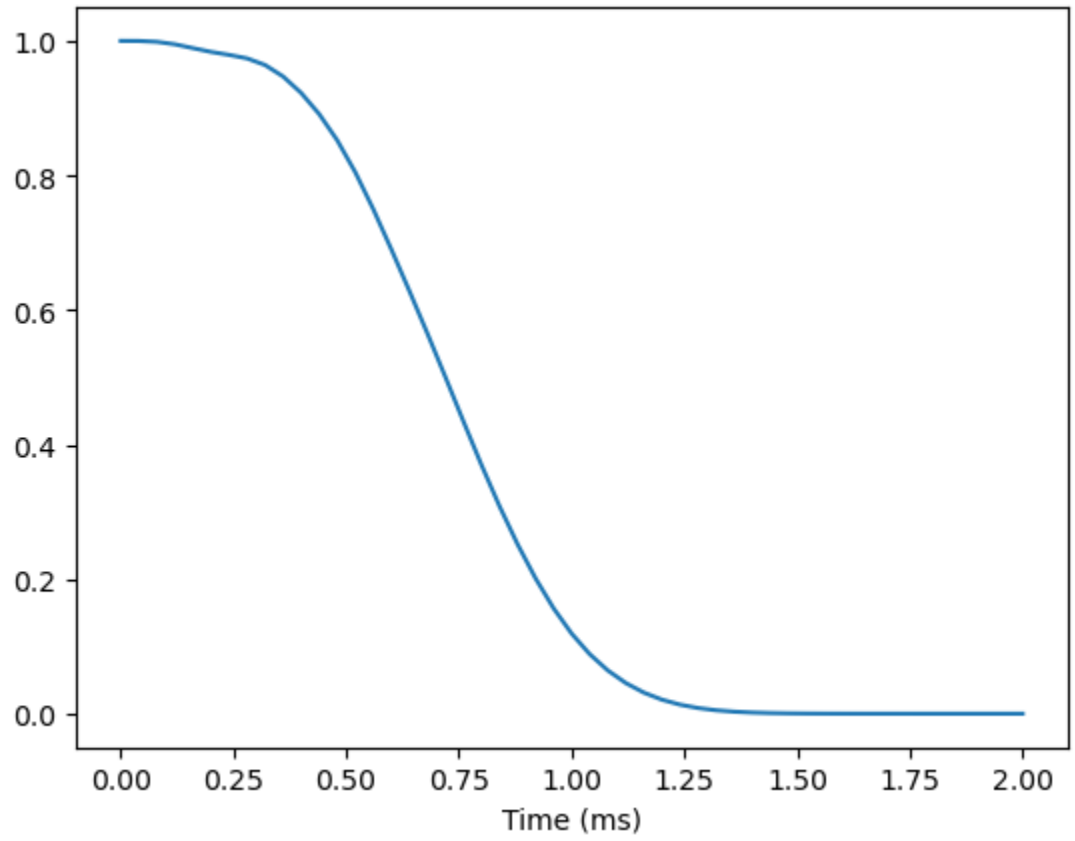
```
calc = pc.Simulator(center, bath=electrons, order=2, r_bath=1.4e3, r_dipole=0.7e3,␣
↪pulses=1, magnetic_field=300, n_clusters=None)
print(calc)
```

```
Simulator for center array of size 1.
magnetic field:
array([  0.,   0., 300.])

Parameters of cluster expansion:
r_bath: 1400.0
r_dipole: 700.0
order: 2

Bath consists of 104 spins.

Clusters include:
104  clusters of order 1.
539  clusters of order 2.
```

As a reference we compute the coherence with conventional CCE assuming no dissipation:

```
ts = np.linspace(0, 2, 51)
lcce = calc.compute(ts, method='cce')
plt.plot(ts, lcce.real)
plt.xlabel('Time (ms)')
```

```
Text(0.5, 0, 'Time (ms)')
```



3.6.2 Dissipation in the bath

In this example we assume that each electron spin in the bath decays into completely random state with the characteristic decay time $T_1 = 0.5$ ms. To add dissipation we use the method `.add_single_jump` method of the `calc.bath` object. Note because we have a single bath type (same name of all spins) the `which` keyword of the method is unnecessary.

```
et1 = 0.5  # in ms
decay_rate = 1 / et1 / 2  # in rad / ms
calc.bath.add_single_jump('p', rate=decay_rate)  # p for creation operator S+
calc.bath.add_single_jump('m', rate=decay_rate)  # m for annihilation operator S-
```

The dissipators are stored in the `.so` attribute of the given spin type in the units of $kHz^{1/2}$ (square root to match how one sets up the simulations in the Qutip, but note that it's not in radial frequencies):

```
calc.bath['e'].so
```

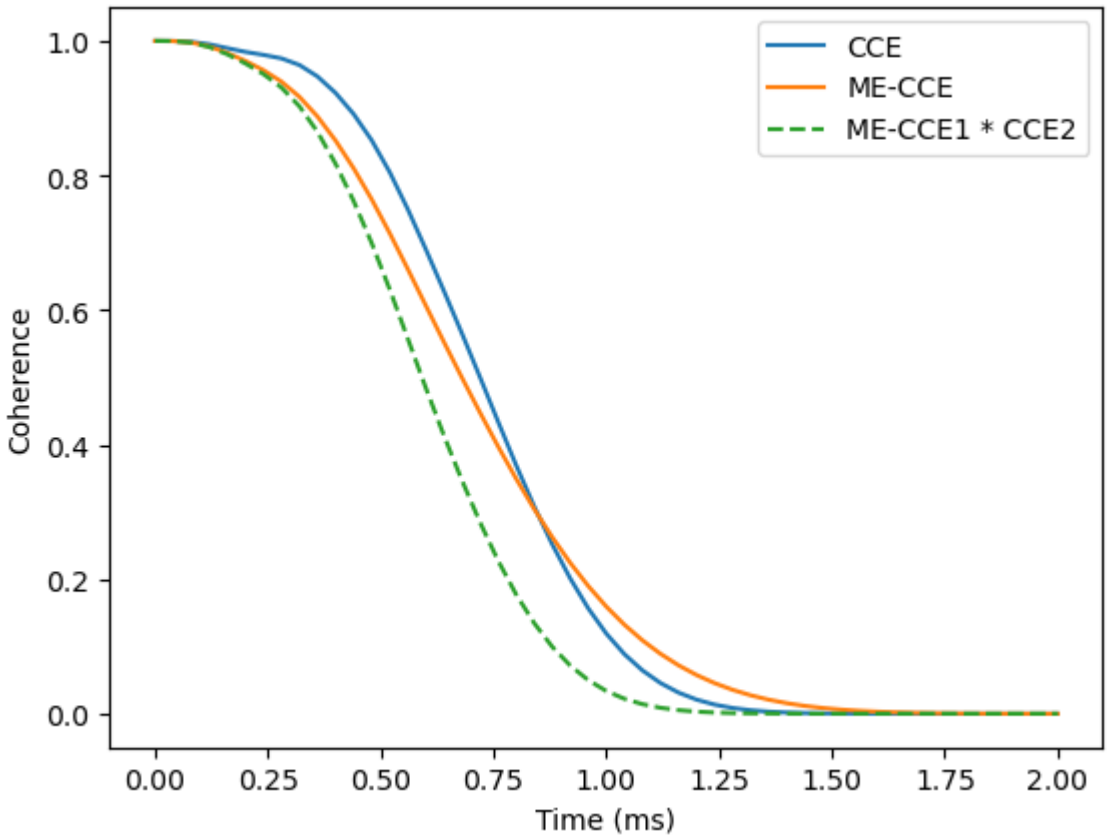
```
{'p': 0.3989422804014327, 'm': 0.3989422804014327}
```

We can compute the coherence with ME-CCE to account for these dissipative dynamics:

```
lmecce = calc.compute(ts, method='mecce')

calc.order = 1
lmecce_1 = calc.compute(ts, method='mecce') # Coherence at first order
```

By comparing the full calculation with ME-CCE to the product of ME-CCE calculation of first order (ME-CCE1) and CCE2 we can directly see the interplay between single spin incoherent dynamics and the coherent flips:

```
plt.plot(ts, lcce.real, label='CCE')
plt.plot(ts, lmecce.real, label='ME-CCE')
plt.plot(ts, (lmecce_1 * lcce).real, ls='--', label='ME-CCE1 * CCE2')

plt.xlabel('Time (ms)')
plt.ylabel('Coherence')

plt.legend();
```



We find that the exact accounting for both coherent and incoherent processes leads to a singificantly different qualitative behaviour of the coherence.

3.6.3 Dissipation in the central spin

To account for the central spin coupling to its own Markovian bath we need to use gCCE flavor of the ME approach.

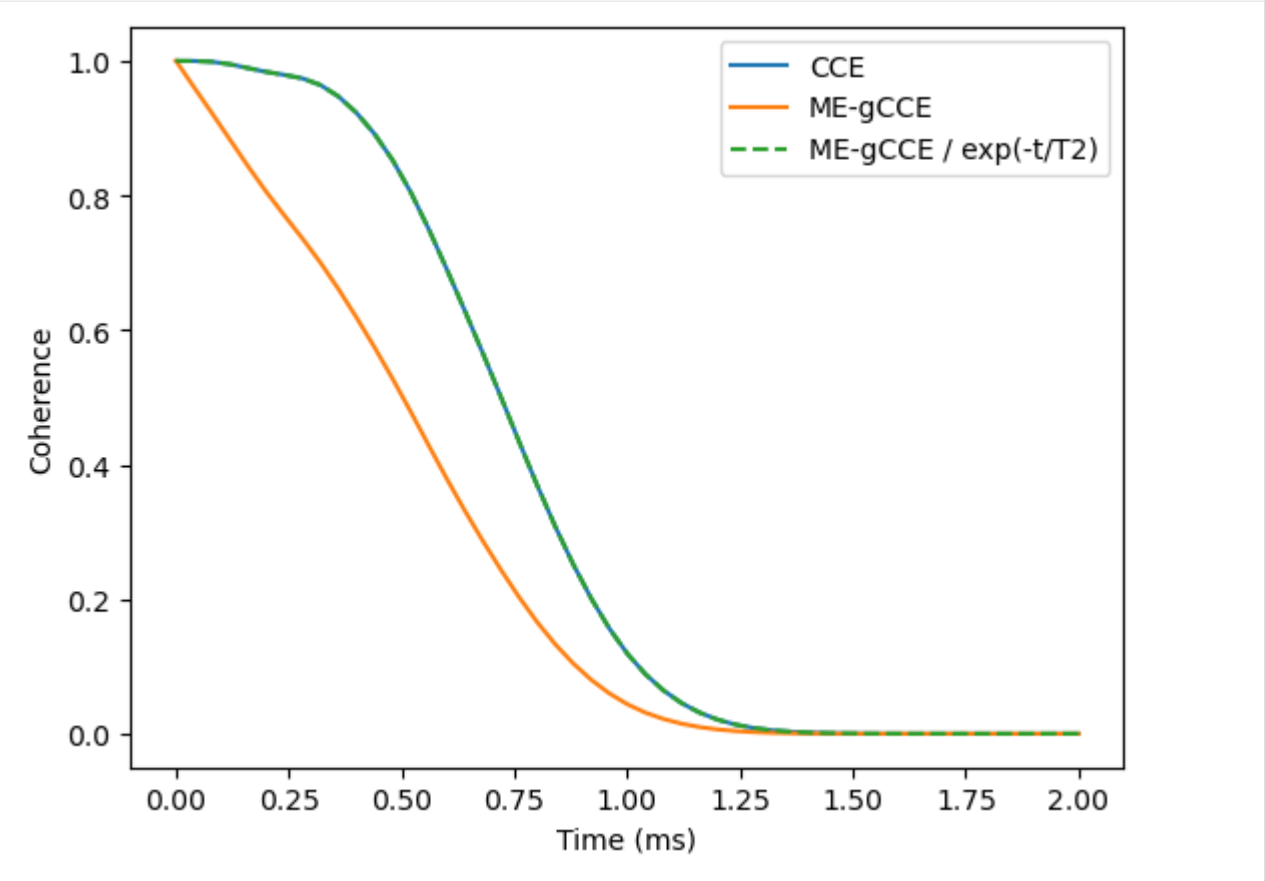
We set up the dissipation on the central spin in the similar way as the bath spins, by calling `.add_single_jump` method of the `calc.center` object. As an example, consider pure dephasing of the central spin due to the Markovian environment.

```
t2 = 1  # in ms
decay_rate = 2 / t2 # in rad / ms
calc.bath['e'].so.clear() # Remove bath spin dissipators
calc.center.add_single_jump('z', rate=decay_rate)  # z for operator Sz
calc.center[0].detuning = 1e6 # Detune central spin from the spin bath
```

```
calc.order = 2
lmegcce = calc.compute(ts, method='megcce', pulses=1)
```

And now we show that central spin dissipators are trivial to deal with and can be factorized out. We can divide the obtained coherence curve by the expected markovian dephasing, and recover the coherence curve limited purely by the interactions with the bath.

```
plt.plot(ts, np.abs(lcce), label='CCE')
plt.plot(ts, np.abs(lmegcce), label='ME-gCCE')
plt.plot(ts, np.abs(lmegcce) / np.exp(-ts/t2), ls='--', label='ME-gCCE / exp(-t/T2)')

plt.xlabel('Time (ms)')
plt.ylabel('Coherence')

plt.legend();
```



Note that calculations with the ME-based methods are significantly more expensive, as we need to solve the eigenvalue problem for the N^4 matrix where N is the size of the Hilbert space, compared to N^2 in the case of the closed system.

The recommended order of the tutorials is from the top to bottom:

- *NV Center in Diamond* example goes through the *Quick Start* example in more details.
- *VV in SiC* tutorial explores the difference between generalized CCE with and without random bath state sampling. Also, in this example we introduce the way to work with DFT output of hyperfine tensors.
- *Shallow donor in Si* example shows the way to include the custom hyperfine couplings for more delocalized defects in semiconductors.
- *Correlation function* example explains the way to use autocorrelation function of the noise to predict the decay of the coherence of the NV center in diamond.
- *Multiple central spins* example goes over the systems with two central spins, either forming a hybrid qubit, or system of two entangled qubits.
- *Dissipative spin bath* example provides details on the master-eqation based solvers ME-CCE and ME-gCCE.

CHAPTER

FOUR

SPIN BATH

4.1 BathArray

Documentation for the `pycce.BathArray` - central class, containing properties of the bath spins.

class BathArray(*shape=None*, *array=None*, *names=None*, *hyperfines=None*, *quadrupoles=None*, *types=None*, *imap=None*, *ca=None*, *sn=None*, *hf=None*, *q=None*, *efg=None*, *state=None*, *center=1*)

Subclass of `ndarray` containing information about the bath spins.

The subclass has fixed structured datatype:

```
_dtype_bath = np.dtype([('N', np.unicode_, 16),
                        ('xyz', np.float64, (3,)),
                        ('A', np.float64, (3, 3)),
                        ('Q', np.float64, (3, 3))])
```

Accessing different fields results in the `ndarray` view.

Each of the fields can be accessed as the attribute of the `BathArray` instance and modified accordingly. In addition to the name fields, the information of the bath spin types is stored in the `types` attribute. All of the items in `types` can be accessed as attributes of the BathArray itself.

Examples

Generate empty `BathArray` instance.

```
>>> ba = BathArray((3,))
>>> print(ba)
[('', [0., 0., 0.], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]], [[0., 0., 0.], [0.,␣
↪0., 0.], [0., 0., 0.]])
 ('', [0., 0., 0.], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]], [[0., 0., 0.], [0.,␣
↪0., 0.], [0., 0., 0.]])
 ('', [0., 0., 0.], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]], [[0., 0., 0.], [0.,␣
↪0., 0.], [0., 0., 0.]])]
```

Generate BathArray from the set of arrays:

```
>>> import numpy as np
>>> ca = np.random.random((2, 3))
>>> sn = ['1H', '2H']
>>> hf = np.random.random((2, 3, 3))
```

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```
>>> ba = BathArray(ca=ca, hf=hf, sn=sn)
>>> print(ba.N, ba.types)
['1H' '2H'] SpinDict(1H: (1H, 0.5, 26.7519), 2H: (2H, 1, 4.1066, 0.00286))
```

Warning: Due to how structured arrays work, if one uses a boolean array to access an subarray, and then access the name field, the initial array *will not change*.

Example:

```
>>> ha = BathArray((10,), sn='1H')
>>> print(ha.N)
['1H' '1H' '1H' '1H' '1H' '1H' '1H' '1H' '1H' '1H']
>>> bool_mask = np.arange(10) % 2 == 0
>>> ha[bool_mask]['N'] = 'e'
>>> print(ha.N)
['1H' '1H' '1H' '1H' '1H' '1H' '1H' '1H' '1H' '1H']
```

To achieve the desired result, one should first access the name field and only then apply the boolean mask:

```
>>> ha['N'][bool_mask] = 'e'
>>> print(ha.N)
['e' '1H' 'e' '1H' 'e' '1H' 'e' '1H' 'e' '1H']
```

Each bath spin can initiallized in some specific state accessing the `.state` attribute. It takes both state vectors and density matrices as values. See `.state` attribute documentation for details.

Parameters

- **shape** (*tuple*) – Shape of the array.
- **array** (*array-like*) – Either an unstructured array with shape (n, 3) containing coordinates of bath spins as rows OR structured ndarray with the same fields as the datatype of the bath.
- **name** (*array-like*) – Array of the bath spin name.
- **hyperfines** (*array-like*) – Array of the hyperfine tensors with shape (n, 3, 3).
- **quadrupoles** (*array-like*) – Array of the quadrupole tensors with shape (n, 3, 3).
- **efg** (*array-like*) – Array of the electric field gradients with shape (n, 3, 3) for each bath spin. Used to compute Quadrupole tensors for spins >= 1. Requires the spin types either be found in `common_isotopes` or specified with `types` argument.
- **types** (`SpinDict`) – SpinDict or input to create one. Contains either SpinTypes of the bath spins or tuples which will initialize those. See `pycce.bath.SpinDict` documentation for details.
- **imap** (`InteractionMap`) – Instance of InteractionMap containing user defined interaction tensors between bath spins stored in the array.
- **ca** (*array-like*) – Shorthand notation for `array` argument.
- **sn** (*array-like*) – Shorthand notation for `name` argument.
- **hf** (*array-like*) – Shorthand notation for `hyperfines` argument.
- **q** (*array-like*) – Shorthand notation for `quadrupoles` argument.

sort(*axis=-1*, *kind=None*, *order=None*)

Sort array in-place. Is implemented only when imap is None. Otherwise use `np.sort`.

property h

Dictionary with additional spin Hamiltonian parameters. Key denotes the product of spin operators as:

Either a string containing `x, y, z, +, -` where each symbol is a corresponding spin operator:

- `x` == S_x
- `y` == S_y
- `z` == S_z
- `p` == S_+
- `m` == S_-

Several symbols is a product of those spin operators.

Or a tuple with indexes (k, q) for Stevens operators (see https://www.easyspin.org/documentation/stevensoperators.html).

The item is the coupling parameter in float.

Examples

- `d['pm'] = 2000` corresponds to the Hamiltonian term $\hat{H}_{add} = A\hat{S}_+\hat{S}_-$ with $A = 2$ MHz.
- `d[2, 0] = 1.5e6` corresponds to Stevens operator $B_k^q\hat{O}_k^q = 3\hat{S}_z - s(s+1)\hat{I}$ with $k = 2$, $q = 0$, and $B_k^q = 1.5$ GHz.

Type
dict

property name

Array of the `name` attribute for each spin in the array from `types` dictionary.

Note: While the value of this attribute should be the same as the `N` field of the BathArray instance, `.name` *should not* be used for production as it creates a *new* array from `types` dictionary.

Type
ndarray

property s

Array of the `spin` (spin value) attribute for each spin in the array from `types` dictionary.

Type
ndarray

property dim

Array of the `dim` (dimensions of the spin) attribute for each spin in the array from `types` dictionary.

Type
ndarray

property gyro

Array of the gyro (gyromagnetic ratio) attribute for each spin in the array from types dictionary.

Type
ndarray

property q

Array of the q (quadrupole moment) attribute for each spin in the array from types dictionary.

Type
ndarray

property detuning

Array of the detuning attribute for each spin in the array from types dictionary.

Type
ndarray

property x

Array of x coordinates for each spin in the array (bath['xyz'][:, 0]).

Type
ndarray

property y

Array of y coordinates for each spin in the array (bath['xyz'][:, 1]).

Type
ndarray

property z

Array of z coordinates for each spin in the array (bath['xyz'][:, 2]).

Type
ndarray

property N

Array of name for each spin in the array (bath['N']).

Type
ndarray

property xyz

Array of coordinates for each spin in the array (bath['xyz']).

Type
ndarray

property A

Array of hyperfine tensors for each spin in the array (bath['A']).

Type
ndarray

property Q

Array of quadrupole tensors for each spin in the array (bath['Q']).

Type
ndarray

property nc

Number of central spins.

Type
int

property state

Array of the bath spin states.

Can have three types of entries:

- **None**. If entry is **None**, assumes fully random density matrix. Default value.
- **ndarray with shape (s,)**. If entry is vector, corresponds to the pure state of the spin.
- **ndarray with shape (s, s)**. If entry is a matrix, corresponds to the density matrix of the spin.

Examples

```
>>> print(ba.state)
[None None]
>>> ba[0].state = np.array([0, 1])
>>> print(ba.state)
[array([0, 1]) None]
```

Type
BathState

property proj

Array of S_z projections of the bath spin states.

Type
ndarray

property has_state

Bool array. True if given spin was initialized with a state, False otherwise.

Type
ndarray

add_type(**args*, ***kwargs*)

Add spin type to the `types` dictionary.

Parameters

- ***args** – Any number of positional inputs to create `SpinDict` entries. E.g. the tuples of form (name `str`, spin `float`, gyro `float`, q `float`).
- ****kwargs** – Any number of keyword inputs to create `SpinDict` entries. E.g. name = (spin, gyro, q).

For details and allowed inputs see `SpinDict` documentation.

Returns
A view of `self.types` instance.

Return type
SpinDict

add_interaction(*i*, *j*, *tensor*)

Add interactions tensor between bath spins with indexes `i` and `j`.

Note: If called from the subarray this method **does not** change the tensors of the total BathArray.

Parameters

- **i** (*int or ndarray (n,)*) – Index of the first spin in the pair or array of the indexes of the first spins in n pairs.
- **j** (*int or ndarray with shape (n,)*) – Index of the second spin in the pair or array of the indexes of the second spins in n pairs.
- **tensor** (*ndarray with shape (3,3) or (n, 3,3)*) – Interaction tensor between the spins i and j or array of tensors.

add_single_jump(*operator*, *rate=1*, *units='rad'*, *square_root=False*, *which=None*)

Add single-spin jump operator for the given type of spins to be used in the Lindbladian master equation CCE.

Parameters

- **operator** (*str or ndarray with shape (dim, dim)*) – Definition of the operator. Can be either of the following: * Pair of integers defining the Sven operator. * String where each symbol corresponds to the spin matrix or operation between them.

  Allowed symbols: `xyz+`. If there is nothing between symbols, assume multiplication of the operators. If there is a + symbol, assume summation between terms. For example, `xx+z` would correspond to the operator $\hat{S}_x\hat{S}_x + \hat{S}_z$.

  – String equal to `A`. Then assumes that the correct matrix form of the operator has been provided by the user.

- **rate** (*float*) – Rate associated with the given jump operator. By default, is given in rad ms^-1.
- **units** (*str*) – Units of the rate, can be either rad (for radial frequency units) or deg (for rotational frequency).
- **square_root** (*bool*) – True if the rate is given as a square root of the rate (to match how one sets up collapse operators in Qutip). Default False.
- **which** (*str*) – For which type of the spins add the jump operator. Default is None - if there is only one spin type in the array then the jump operator is added, otherwise the exception is raised.

update(*ext_bath*, *error_range=0.2*, *ignore_isotopes=True*, *inplace=True*)

Update the properties of the spins in the array using data from other `BathArray` instance. For each spin in `ext_bath` check whether there is such spin in the array that has the same position within allowed error range given by `error_range` and has the same name. If such spins is found in the array, then it's coordinates, hyperfine tensor and quadrupole tensor are updated using the values of the spin in the `ext_bath` object.

If `ignore_isotopes` is true, then the name check ignores numbers in the name of the spins.

Parameters

- **ext_bath** (BathArray) – Array of the new spins.

- **error_range** (*float*) – +- distance in Angstrom within which two positions are considered to be the same. Default is 0.2 A.
- **ignore_isotopes** (*bool*) – True if ignore numbers in the name of the spins. Default True.
- **inplace** (*bool*) – True if changes parameters of the array in place. If False, returns copy of the array.

Returns
updated BathArray instance.

Return type
BathArray

from_center(*center*, *inplace=True*, *cube=None*, *which=0*, ***kwarg*)

Generate hyperfine couplings using either the point dipole approximation or spin density in the .cube format, with the information from the CenterArray instance.

Parameters

- **center** (CenterArray) – Array, containing properties of the central spin
- **inplace** (*bool*) – True if changes parameters of the array in place. If False, returns copy of the array.
- **cube** (Cube *or iterable of Cubes*) – An instance of Cube object, which contains spatial distribution of spin density of central spins. For details see documentation of Cube class.
- **which** (*int*) – If cube is a single Cube instance, this is an index of the central spin it corresponds to.
- ****kwarg** – Additional arguments for .from_cube method.

Returns
Updated BathArray instance.

Return type
BathArray

from_point_dipole(*position*, *gyro_center=-17608.59705*, *inplace=True*)

Generate hyperfine couplings, assuming that bath spins interaction with central spin is the same as the one between two magnetic point dipoles.

Parameters

- **position** (*ndarray with shape (3,)*) – position of the central spin
- **gyro_center** (*float or ndarray with shape (3,3)*) – gyromagnetic ratio of the central spin

  OR

  tensor corresponding to interaction between magnetic field and central spin.
- **inplace** (*bool*) – True if changes parameters of the array in place. If False, returns copy of the array.

Returns
Updated BathArray instance with changed hyperfine couplings.

Return type
BathArray

from_cube(*cube*, *gyro_center=-17608.59705*, *inplace=True*, *which=0*, ***kwargs*)

Generate hyperfine couplings, assuming that bath spins interaction with central spin can be approximated as a point dipole, interacting with given spin density distribution.

Parameters

- **cube** (Cube) – An instance of *Cube* object, which contains spatial distribution of spin density. For details see documentation of *Cube* class.
- **gyro_center** (*float*) – Gyromagnetic ratio of the central spin.
- **inplace** (*bool*) – True if changes parameters of the array in place. If False, returns copy of the array.

Returns

Updated BathArray instance with changed hyperfine couplings.

Return type

BathArray

from_func(*func*, **args*, *inplace=True*, ***kwargs*)

Generate hyperfine couplings from user-defined function.

Parameters

- **func** (*func*) – Callable with signature:

```
func(array, *args, **kwargs)
```

  where `array` is array of the bath spins,

- ***args** – Positional arguments of the `func`.
- ****kwargs** – Keyword arguments of the `func`.
- **inplace** (*bool*) – True if changes parameters of the array in place. If False, returns copy of the array.

Returns

Updated BathArray instance with changed hyperfine couplings.

Return type

BathArray

from_efg(*efg*, *inplace=True*)

Generate quadrupole splittings from electric field gradient tensors for spins >= 1.

Parameters

- **efg** (*array-like*) – Array of the electric field gradients for each bath spin. The data for spins-1/2 should be included but can be any value.
- **inplace** (*bool*) – True if changes parameters of the array in place. If False, returns copy of the array.

Returns

Updated BathArray instance with changed quadrupole tensors.

Return type

BathArray

dist(*position=None*)

Compute the distance of the bath spins from the given position.

Parameters
position (*ndarray with shape (3,)*) – Cartesian coordinates of the position from which to compute the distance. Default is (0, 0, 0).

Returns
Array of distances of each bath spin from the given position in angstrom.

Return type
ndarray with shape (n,)

savetxt(*filename*, *fmt='%18.8f'*, *strip_isotopes=False*, ***kwargs*)

Save name of the isotopes and their coordinates to the txt file of xyz format.

Parameters

- **filename** (*str or file*) – Filename or file handle.
- **fmt** (*str*) – Format of the coordinate entry.
- **strip_isotopes** (*bool*) – True if remove numbers from the name of bath spins. Default False.
- ****kwargs** – Additional keywords of the `numpy.savetxt` function.

sort(*a*, *axis=-1*, *kind=None*, *order=None*)

Return a sorted copy of an array. Overrides numpy.sort function.

argsort(*a*, **args*, ***kwargs*)

Return a indexes of a sorted array. Overrides `numpy.argsort` function.

check_gyro(*gyro*)

Check if gyro is matrix or scalar.

Parameters
gyro (*ndarray or float*) – Gyromagnetic ratio matrix or float.

Returns

tuple containing:

- **ndarray or float**: Gyromagnetic ratio.
- **bool**: True if gyro is float, False otherwise.

Return type
tuple

point_dipole(*pos*, *gyro_array*, *gyro_center*)

Generate an array hyperfine couplings, assuming point dipole approximation.

Parameters

- **pos** (*ndarray with shape (n, 3)*) – Relative position of the bath spins.
- **gyro_array** (*ndarray with shape (n,)*) – Array of the gyromagnetic ratios of the bath spins.
- **gyro_center** (*float or ndarray with shape (3, 3)*) – gyromagnetic ratio of the central spin

  OR

tensor corresponding to interaction between magnetic field and central spin.

Returns
Array of hyperfine tensors.

Return type
ndarray with shape (n, 3, 3)

same_bath_indexes(*barray_1*, *barray_2*, *error_range=0.2*, *ignore_isotopes=True*)

Find indexes of the same array elements in two `BathArray` instances.

Parameters

- **barray_1** (`BathArray`) – First array.
- **barray_2** (`BathArray`) – Second array.
- **error_range** (*float*) – If distance between positions in two arrays is smaller than `error_range` they are assumed to be the same.
- **ignore_isotopes** (*bool*) – True if ignore numbers in the name of the spins. Default True.

Returns

tuple containing:

- **ndarray**: Indexes of the elements in the first array found in the second.
- **ndarray**: Indexes of the elements in the second array found in the first.

Return type
tuple

broadcast_array(*array*, *root=0*)

Using mpi4py broadcast `BathArray` or `CenterArray` to all processes. :param array: Array to broadcast. :type array: BathArray or CenterArray :param root: Rank of the process to broadcast from. :type root: int

Returns
Broadcasted array.

Return type
BathArray or *CenterArray*

utilities.**rotmatrix**(*final_vector*)

Generate 3D rotation matrix which applied on initial vector will produce vector, aligned with final vector.

Examples

```
>>> R = rotmatrix([0,0,1], [1,1,1])
>>> R @ np.array([0,0,1])
array([0.577, 0.577, 0.577])
```

Parameters

- **initial_vector** (*ndarray with shape(3,)*) – Initial vector.
- **final_vector** (*ndarray with shape (3,)*) – Final vector.

Returns
Rotation matrix.

Return type
ndarray with shape (3, 3)

4.1.1 BathState

class BathState(*size*)

Class for storing the state of the bath spins. Usually is not generated directly, but accessed as an `BathArray.state` attribute.

Parameters
size (*int*) – Number of bath states to be stored.

gen_pure(*rho*, *dim*)

Generate pure states from the S_z projections to be stored in the given `BathState` object.

Parameters

- **rho** (*ndarray with shape (n,)*) – Array of the desired projections.
- **dim** (*ndarray with shape (n,)*) – Array of the dimensions of the spins.

Returns
View of the `BathState` object.

Return type
BathState

property state

Return an underlying object array.

Type
ndarray

property pure

Bool property. True if given entry is a pure state, False otherwise.

Type
ndarray

property proj

Projections of bath states on S_z.

Type
ndarray

property has_state

Bool property. True if given element was initialized as a state, False otherwise.

Type
ndarray

project(*rotation=None*)

Generate projections of bath states on S_z.

Parameters
rotation (*optional, ndarray with shape (3, 3)*) – Matrix used to transform S_z matrix as $S_z' = R^\dagger S_z R$.

Returns
Array with projections of the state.

Return type
ndarray with shape (n,)

property shape

Shape of the BathState underlying array.

Type
tuple

property size

Size of the BathState underlying array.

Type
int

any(**args*, ***kawrgs*)

Returns the output of `.has_state.any` method. :param *args: Positional arguments of `.has_state.any` method. :param **kawrgs: Keyword arguments of `.has_state.any` method.

Returns
True if any entry is initialized. Otherwise False.

Return type
bool

4.1.2 Cube

class Cube(*filename*)

Class to process the .cube datafiles with spin polarization.

Parameters
filename (*str*) – Name of the .cube file.

comments

First two lines of the .cube file.

Type
str

origin

Coordinates of the origin in angstrom.

Type
ndarray with shape (3,)

voxel

Parameters of the voxel - unit of the 3D grid in angstrom.

Type
ndarray with shape (3,3)

size

Size of the cube.

Type
ndarray with shape (3,)

atoms

Array of atoms in the cube.

Type
BathArray with shape (n)

data

Data stored in cube.

Type
ndarray with shape (size[0], size[1], size[2]

grid

Coordinates of the points at which data is computed.

Type
ndarray with shape (size[0], size[1], size[2], 3

integral

Data integrated over cube.

Type
float

spin

integral / 2 - total spin.

Type
float

transform(*rotmatrix=None*, *shift=None*)

Changes coordinates of the grid. DOES NOT ASSUME PERIODICITY.

Parameters

- **rotmatrix** (*ndarray with shape (3, 3)*) – Rotation matrix *R*:

$$R = [n_1^{(1)} n_1^{(2)} n_1^{(3)}]$$
$$[n_2^{(1)} n_2^{(2)} n_2^{(3)}]$$
$$[n_3^{(1)} n_3^{(2)} n_3^{(3)}]$$

  where $n_i^{(j)}$ corresponds to the coefficient of initial basis vector i for j new basis vector:

$$e'_j = n_1^{(j)}\vec{e}_1 + n_2^{(j)}\vec{e}_2 + n_3^{(j)}\vec{e}_3$$

  In other words, columns of *R* are coordinates of the new basis in the old basis.

  Given vector in initial basis v = [v1, v2, v3], vector in new basis is given as v' = R.T @ v.

- **shift** (*ndarray with shape (3,)*) – Shift in the origin of coordinates (in the old basis).

integrate(*position*, *gyro_n*, *gyro_e=-17608.59705*, *spin=None*, *parallel=False*, *root=0*)

Integrate over polarization data, stored in Cube object, to obtain hyperfine dipolar-dipolar tensor.

Parameters

- **position** (*ndarray with shape (3,) or (n, 3)*) – Position of the bath spin at which to compute hyperfine tensor or array of positions.
- **gyro_n** (*float or ndarray with shape (n,)*) – Gyromagnetic ratio of the bath spin or array of the ratios.
- **gyro_e** (*float*) – Gyromagnetic ratio of central spin.
- **spin** (*float*) – Total spin of the central spin. If not given, taken from the integral of the polarization.

Returns
Hyperfine tensor or array of hyperfine tensors.

Return type
ndarray with shape (3, 3) or (n, 3, 3)

4.1.3 SpinDict and SpinType

Documentation for the `SpinDict` - dict-like class which describes the properties of the different types of the spins in the bath.

class SpinDict(**args*, ***kwargs*)

Wrapper class for dictionary tailored for containing properties of the spin types. Can take `np.void` or `BathArray` instances as keys. Every entry is instance of the `SpinType`.

Each entry of the `SpinDict` can be initianlized as follows:

- As a Tuple containing name (optional), spin, gyromagnetic ratio, quadrupole constant (optional) and detuning (optional).
- As a `SpinType` instance.

Examples

```
>>> types = SpinDict()
>>> types['1H'] = ('1H', 1 / 2, 26.7519)
>>> types['2H'] = 1, 4.1066, 0.00286
>>> types['3H'] = SpinType('3H', 1 / 2, 28.535, 0)
>>> print(types)
SpinDict({'1H': (1H, 0.5, 26.7519, 0.0), '2H': (2H, 1, 4.1066, 0.00286), '3H': (3H,␣
↪0.5, 28.535, 0)})
```

If `SpinType` of the given bath spin is not provided, when requested `SpinDict` will try to find information about the bath spins in the `common_isotopes`.

If found, adds an entry to the given `SpinDict` instance and returns it. Otherwise `KeyError` is raised.

To initiallize several `SpinType` entries one can use `add_types` method.

Parameters

- ***args** – Any numbers of arguments which could initialize `SpinType` instances.
- ****kwargs** – Any numbers of keyword arguments which could initialize `SpinType` instances. For details see `SpinDict.add_type` method.

add_type(**args*, ***kwargs*)

Add one or several spin types to the spin dictionary.

Parameters

- ***args** – Any numbers of arguments which could initialize `SpinType` instances. Accepted arguments:
  - Tuple containing name, spin, gyromagnetic ratio, quadrupole constant (optional) and detuning (optional).
  - `SpinType` instance.

Can also initialize one instance of `SpinType` if each argument corresponds to each positional argument necessary to initiallize.

- **`**kwargs`** – Any numbers of keyword arguments which could initialize `SpinType` instances. Usefull as an alternative for updating the dictionary. for each keyword argument adds an entry to the `SpinDict` with the same name as keyword.

Examples

```
>>> types = SpinDict()
>>> types.add_type('1H', 1 / 2, 26.7519)
>>> types.add_type(('1H_det', 1 / 2, 26.7519, 10), ('2H', 1, 4.1066, 0.00286),
>>>                SpinType('3H', 1 / 2, 28.535, 0), e=(1 / 2, 6.7283, 0))
>>> print(types)
SpinDict(1H: (1H, 0.5, 26.7519), 1H_det: (1H_det, 0.5, 26.7519, 10),
2H: (2H, 1, 4.1066, 0.00286), 3H: (3H, 0.5, 28.535), e: (e, 0.5, 6.7283))
```

class SpinType(*name*, *s=0.0*, *gyro=0.0*, *q=0.0*, *detuning=0.0*)

Class which contains properties of each spin type in the bath.

Parameters

- **`name`** (*`str`*) – Name of the bath spin.
- **`s`** (*`float`*) – Total spin of the bath spin.

  Default 0.
- **`gyro`** (*`float`*) – Gyromagnetic ratio in rad * kHz / G.

  Default 0.
- **`q`** (*`float`*) – Quadrupole moment in barn (for s > 1/2).

  Default 0.
- **`detuning`** (*`float`*) – Energy detuning from the zeeman splitting in kHz, included as an extra $+\omega\hat{S}_z$ term in the Hamiltonian, where ω is the detuning.

  Default 0.

`name`

Name of the bath spin.

Type
str

`s`

Total spin of the bath spin.

Type
float

`dim`

Spin dimensionality = 2s + 1.

Type
int

gyro

Gyromagnetic ratio in rad/(ms * G).

Type
float

q

Quadrupole moment in barn (for s > 1/2).

Type
float

detuning

Energy detuning from the zeeman splitting in kHz.

Type
float

property h

Dictionary with additional spin Hamiltonian parameters. Key denotes the product of spin operators as:

Either a string containing `x, y, z, +, -` where each symbol is a corresponding spin operator:

- `x` == S_x
- `y` == S_y
- `z` == S_z
- `p` == S_+
- `m` == S_-

Several symbols is a product of those spin operators.

Or a tuple with indexes (k, q) for Stevens operators (see https://www.easyspin.org/documentation/stevensoperators.html).

The item is the coupling parameter in float.

Examples

- `d['pm'] = 2000` corresponds to the Hamiltonian term $\hat{H}_{add} = A\hat{S}_+\hat{S}_-$ with $A = 2$ MHz.
- `d[2, 0] = 1.5e6` corresponds to Stevens operator $B_k^q\hat{O}_k^q = 3\hat{S}_z - s(s+1)\hat{I}$ with $k = 2$, $q = 0$, and $B_k^q = 1.5$ GHz.

Type
dict

common_isotopes = SpinDict(1H: (0.5, 26.7522), 2H: (1.0, 4.1066, 0.0029), 3He: (0.5, -20.3789), ...)

An instance of the `SpinDict` dictionary, containing properties for the most of the common isotopes with nonzero spin. The isotope is considered common if it is stable and has nonzero concentration in nature.

Type
SpinDict

common_concentrations = {element ('H', 'He',...) : { isotope ('1H', '2H', ..) : concentration}}

Nested dict containing natural concentrations of the stable nuclear isotopes.

Type
dict

4.2 Random bath

Documentation for the `pycce.random_bath` function, used to generate random bath.

random_bath(*names*, *size*, *number=1000*, *density=None*, *types=None*, *density_units='cm-3'*, *center=None*, *seed=None*)

Generate random bath containing spins with names provided with argument `name` in the box of size `size`. By default generates coordinates in range (-size/2; +size/2) but this behavior can be changed by providing `center` keyword.

Examples

Generate 2000 ^{13}C nuclear spins in the cubic box with the side of 100 angstrom:

```
>>> atoms = random_bath('13C', 100, number=2000, seed=10)
>>> print(atoms.size)
2000
>>> print(round(atoms.x.min()), round(atoms.x.max()))
-50.0 50.0
```

Generate electron spin bath with density $10^{17}\mathrm{cm}^{-3}$ in the cuboid box:

```
>>> electrons = random_bath('e', [1e3, 2e3, 3e3], density=1e17,
>>>                         density_units='cm-3', seed=10)
>>> print(electrons.size, round(electrons.x.min()), round(electrons.x.max()))
600 -494.0 500.0
>>> print(electrons.types)
SpinDict(e: (e, 0.5, -17608.59705))
```

Parameters

- **names** (*str or array-like with length n*) – Name of the bath spin or array with the names of the bath spins,
- **size** (*float or ndarray with shape (3,)*) – Size of the box. If float is given, assumes 3D cube with the edge = `size`. Otherwise the size specifies the dimensions of the box. Dimensionality is controlled by setting entries of the size array to 0.
- **number** (*int or array-like with length n*) – Number of the bath spins in the box or array with the numbers of the bath spins. Has to have the same length as the `name` array.
- **density** (*float or array-like with length n*) – Concentration of the bath spin or array with the concentrations. Has to have the same length as the `name` array.
- **types** (SpinDict) – Dictionary with SpinTypes or input to create one.

- **density_units** (*str*) – If number of spins provided as density, defines units. Values are accepted in the format `m`, or `m^x` or `m-x` where m is the length unit, x is dimensionality of the bath (e.g. x = 1 for 1D, 2 for 2D etc). If only `m` is provided the dimensions are inferred from `size` argument. Accepted length units:
  - `m` meters;
  - `cm` centimeters;
  - `a` angstroms.
- **center** (*ndarray with shape (3,)*) – Coordinates of the (0, 0, 0) point of the final coordinate system in the initial coordinates. Default is `size / 2` - center is in the middle of the box.
- **seed** (*int*) – Seed for random number generator.

Returns
Array of the bath spins with random positions.

Return type
BathArray with shape (np.prod(number),)

4.3 BathCell

Documentation for the `pycce.BathCell` - class for convenient generation of `BathArray` and the necessary helper functions.

class BathCell(*a=None*, *b=None*, *c=None*, *alpha=None*, *beta=None*, *gamma=None*, *angle='rad'*, *cell=None*)

Generator of the bath spins positions from the unit cell of the material.

Parameters

- **a** (*float*) – a parameter of the primitive cell.
- **b** (*float*) – b parameter of the primitive cell.
- **c** (*float*) – c parameter of the primitive cell.
- **alpha** (*float*) – α angle of the primitive cell.
- **beta** (*float*) – β angle of the primitive cell.
- **gamma** (*float*) – γ angle of the primitive cell.
- **angle** (*str*) – units of the α, β, γ angles. Can be either radians (`'rad'`), or degrees (`'deg'`).
- **cell** (*ndarray with shape (3, 3)*) – Parameters of the cell.

  `cell` is 3x3 matrix with columns of coordinates of crystallographic vectors in the cartesian reference frame. See `cell` attribute.

  If provided, overrides *a*, *b*, and *c*.

cell

Parameters of the cell. `cell` is 3x3 matrix with entries:

$$[[a_x\ b_x\ c_x]$$
$$[a_y\ b_y\ c_y]$$
$$[a_z\ b_z\ c_z]]$$

where a, b, c are crystallographic vectors and x, y, z are their coordinates in the cartesian reference frame.

Type
ndarray with shape (3, 3)

`atoms`

Dictionary containing coordinates and occupancy of each lattice site:

```
{atom_1: [array([x1, y1, z1]), array([x2, y2, z2])],
 atom_2: [array([x3, y3, z3]), ...]}
```

Type
dict

`isotopes`

Dictionary containing spin types and their concentration for each lattice site type:

```
{atom_1: {spin_1: concentration, spin_2: concentration},
 atom_2: {spin_3: concentration ...}}
```

where `atom_i` are lattice site types, and `spin_i` are spin types.

Type
dict

`property zdir`

z-direction of the reference cartesian coordinate frame in cell coordinates.

Type
ndarray

`rotate`(*rotation_matrix*)

Rotate the BathCell using the rotation matrix provided.

Parameters
rotation_matrix (*ndarray with shape (3,)*) – Rotation matrix R which rotates the old basis of the cartesian reference frame to the new basis.

`set_zdir`(*direction*, *type='cell'*)

Set z-direction of the cell.

Parameters

- **direction** (*ndarray with shape (3,)*) – Direction of the z axis.
- **type** (*str*) – How coordinates in `direction` are stored. If `type="cell"`, assumes crystallographic coordinates. If `type="angstrom"` assumes that z direction is given in the cartresian reference frame.

`add_atoms`(**args*, *type='cell'*)

Add coordinates of the lattice sites to the unit cell.

Parameters

- ***args** (*tuple*) – List of tuples, each containing the type of atom N (*str*), and the xyz coordinates in the format (*float, float, float*): `(N, [x, y, z])`.
- **type** (*str*) – Type of coordinates. Can take values of `['cell', 'angstrom']`.

  If `type="cell"`, assumes crystallographic coordinates.

  If `type="angstrom"` assumes that coordinates are given in the cartresian reference frame.

Returns
View of `cell.atoms` dictionary, where each key is the type of lattice site, and each value is the list of coordinates in crystallographic frame.

Return type
dict

Examples

```
>>> cell = BathCell(10)
>>> cell.add_atoms(('C', [0, 0, 0]), ('C', [5, 5, 5]), type='angstrom')
>>> cell.add_atoms(('Si', [0, 0.5, 0.]), type='cell')
>>> print(cell.atoms)
{'C': [array([0., 0., 0.]), array([0.5, 0.5, 0.5])], 'Si': [array([0. , 0.5, 0.␣
↪])]}
```

add_isotopes(**args*)

Add spins that can populate each lattice site type.

Parameters
***args** (*tuple or list of tuples*) – Each tuple can have any of the following formats:

- Name of the lattice site *N* (*str*), name of the spin *X* (*str*), concentration *c* (*float*, in decimal): `(N, X, c)`.
- Isotope name *X and concentration `c*: `(X, c)`.

  In this case, the name of the isotope is given in the format `"{}{}".format(digits, atom_name)` where `digits` is any set of digits 0-9, `atom_name` is the name of the corresponding lattice site. Convenient when generating nuclear spin bath.

Returns

View of `cell.isotopes` dictionary which contains information about lattice site types, spin types, and their concentrations:

```
{atom_1: {spin_1: concentration, spin_2: concentration},
 atom_2: {spin_3: concentration ...}}
```

Return type
dict

Examples

```
>>> cell = BathCell(10)
>>> cell.add_atoms(('C', [0, 0, 0]), ('C', [5, 5, 5]), type='angstrom')
>>> cell.add_isotopes(('C', 'X', 0.001), ('13C', 0.0107))
>>> print(cell.isotopes)
{'C': {'X': 0.001, '13C': 0.0107}}
```

gen_supercell(*size*, *add=None*, *remove=None*, *seed=None*, *recenter=True*)

Generate supercell populated with spins.

Note: If `isotopes` were not provided, assumes the natural concentration of nuclear spin isotopes for each lattice site type. However, if any isotope concentration is provided, then uses only user-defined ones.

Parameters

- **size** (*float*) – Approximate linear size of the supercell. The generated supercell will have minimal distance between opposite sides larger than this parameter.
- **add** (*tuple or list of tuples*) – Tuple or list of tuples containing common_isotopes to add as a defect. Each tuple contains name of the new isotope and its coordinates in the cell basis: `(isotope_name, x_cell, y_cell, z_cell)`.
- **remove** (*tuple or list of tuples*) – Tuple or list of tuples containing bath to remove in the defect. Each tuple contains name of the atom to remove and its coordinates in the cell basis: `(atom_name, x_cell, y_cell, z_cell)`.
- **seed** (*int*) – Seed for random number generator.
- **recenter** (*bool*) – True if place approximate center of the supercell at (0,0,0). False if start supercell at (0, 0, 0). Default True.

Note: While `add` takes the **spin** name as an argument, `remove` takes the lattice site name.

Returns
Array of the spins in the given supercell.

Return type
BathArray

`to_cartesian`(*coord*)

Transform coordinates from crystallographic basis to the cartesian reference frame.

Parameters
coord (*ndarray with shape (3,) or (n, 3)*) – Coordinates in crystallographic basis or array of coordinates.

Returns
Cartesian coordinates in angstrom.

Return type
ndarray with shape (3,) or (n, 3)

`to_cell`(*coord*)

Transform coordinates from the cartesian coordinates of the reference frame to the cell coordinates.

Parameters
coord (*ndarray with shape (3,) or (n, 3)*) – Cartesian coordinates in angstrom or array of coordinates.

Returns
Coordinates in the cell basis.

Return type
ndarray with shape (3,) or (n, 3)

classmethod from_ase(*atoms_object*)

Generate `BathCell` instance from `ase.Atoms` object of Atomic Simulations Environment (ASE) package.

Parameters
atoms_object (*Atoms*) – Atoms object, used to generate new `BathCell` instance.

Returns
New instance of the `BathCell` with atoms read from `ase.Atoms`.

Return type
BathCell

read_ase(*atoms_object*)

Generate `BathCell` instance from `ase.Atoms` object of Atomic Simulations Environment (ASE) package.

Parameters
atoms_object (*Atoms*) – Atoms object, used to generate new `BathCell` instance.

Returns
New instance of the `BathCell` with atoms read from `ase.Atoms`.

Return type
BathCell

defect(*cell*, *atoms*, *add=None*, *remove=None*)

Generate a defect in the given supercell.

The defect will be located in the unit cell, located roughly in the middle of the supercell, generated by `BathCell`, such that (0, 0, 0) of cartesian reference frame is located at (0, 0, 0) position of this unit cell.

Parameters

- **cell** (*ndarray with shape (3, 3)*) – parameters of the unit cell.
- **atoms** (`BathArray`) – Array of spins in the supercell.
- **add** (*tuple or list of tuples*) – Add spin type(s) to the supercell at specified positions to create point defect. Each tuple contains name of the new isotope and its coordinates in the cell basis: `(isotope_name, x_cell, y_cell, z_cell)`.
- **remove** (*tuple or list of tuples*) – Remove lattice site from the supercell at specified position to create point defect. Each tuple contains name of the atom to remove and its coordinates in the cell basis: `(atom_name, x_cell, y_cell, z_cell)`.

Returns
Array of spins with the defect added.

Return type
BathArray

CHAPTER

FIVE

CENTRAL SPINS

5.1 CenterArray

Documentation for the `pycce.CenterArray` - class which stores the properties of the set of central spins.

class CenterArray(*size=None*, *position=None*, *spin=None*, *D=0*, *E=0*, *gyro=-17608.59705*, *imap=None*, *alpha=None*, *beta=None*, *detuning=0*)

Class, containing properties of all central spins. The properties of the each separate spin can be accessed as elements of the object directly. Each element of the array is an instance of the `Center` class.

Examples

Generate array of 2 electron central spins:

```
>>> import numpy as np
>>> ca = CenterArray(2, spin=0.5) # Array of size 2 with spins-1/2
>>> print(ca)
CenterArray
(s: [0.5 0.5],
xyz:
[[0. 0. 0.]
 [0. 0. 0.]],
zfs:
[[[0. 0. 0.]
  [0. 0. 0.]
  [0. 0. 0.]]
 [[0. 0. 0.]
  [0. 0. 0.]
  [0. 0. 0.]]],
gyro:
[[[-17608.59705     -0.          -0.     ]
  [    -0.      -17608.59705     -0.     ]
  [    -0.          -0.      -17608.59705]]
 [[-17608.59705     -0.          -0.     ]
  [    -0.      -17608.59705     -0.     ]
  [    -0.          -0.      -17608.59705]]])
```

Set first two eigenstates of the combined central spin Hamiltonian as a singlie qubit state:

```
>>> ca.alpha = 0
>>> ca.beta = 1
```

Change gyromagnetic ratio of the first spin:

```
>>> ca[0].gyro = np.eye(3) * 1000
>>> print(ca[0])
Center
(s: 0.5,
xyz:
[0. 0. 0.],
zfs:
[[0. 0. 0.]
 [0. 0. 0.]
 [0. 0. 0.]],
gyro:
1000.0)
```

Parameters

- **size** (*int*) – Number of central spins.
- **spin** (*ndarray with shape (size,)*) – Total spins of the central spins.

  Note: All center spin properties are broadcasted to the total size of the center array, provided by `size` argument, or inferred from `spin`, `position` arguments.

- **position** (*ndarray with shape (size, 3)*) – Cartesian coordinates in Angstrom of the central spins. Default (0., 0., 0.).
- **D** (*ndarray with shape (size,) or ndarray with shape (n, 3, 3)*) – D (longitudinal splitting) parameters of central spins in ZFS tensor of central spin in kHz.

  OR

  Total ZFS tensor. Default 0.

- **E** (*ndarray with shape (size,)*) – E (transverse splitting) parameters of central spins in ZFS tensor of central spin in kHz. Default 0. Ignored if `D` is None or tensor.
- **gyro** (*ndarray with shape (size,) or ndarray with shape (size, 3, 3)*) – Gyromagnetic ratios of the central spins in rad / ms / G.

  OR

  Tensors describing central spins interactions with the magnetic field.

  Default -17608.597050 kHz * rad / G - gyromagnetic ratio of the free electron spin.

- **imap** (*dict or InteractionMap or ndarray with shape (3, 3)*) – Dict-like object containing interaction tensors between the central spins of the structure {(i, j): T_ij}. Where i, j are positional indexes of the central spins. If provided as an ndarray with shape (3, 3), assumes the same interactions between all pairs of central spins in the array. If provided with shape (size * (size - 1) / 2, 3, 3), assigns the interactions to the ordered pairs: `{(0, 1): imap[0], (0, 2): imap[1] ... (size - 2, size - 1): imap[-1]}`
- **alpha** (*int or ndarray with shape (S,)*) – 0 state of the qubit in the product space of all central spins, or the index of eigenstate to be used as one.

  Default is **None**.

- **beta** (*int or ndarray with shape (S,)*) – 1 state of the qubit in the product space of all central spins, or the index of eigenstate to be used as one.

Default is **None**.

- **detuning** (*ndarray with shape (size,)*) – Energy detunings from the Zeeman splitting in kHz, included as an extra $+\omega\hat{S}_z$ term in the Hamiltonian, where ω is the detuning.

  Default is 0.

energy_alpha

Energy of the alpha state. Generated by `.generate_projections` call if `second_order=True`.

Type
float

energy_beta

Energy of the beta state. Generated by `.generate_projections` call if `second_order=True`.

Type
float

energies

Energy of each eingenstate of the central spin Hamiltonian.

Type
ndarray with shape (n,)

property imap

dict-like object, which contains interactions between central spins.

Type
InteractionMap

property alpha

0 qubit state of the central spin in S_z basis

OR index of the energy state to be considered as one.

If not provided in the `CentralArray` instance, returns the tensor product of all `alpha` states of each element of the array. If there are undefined `alpha` states of the elements of the array, raises an error.

Examples

```
>>> ca = CenterArray(2, spin=0.5) # Array of size 2 with spins-1/2
>>> ca[0].alpha = [0,1]
>>> ca[1].alpha = [1,0]
>>> print(ca.alpha)
[0.+0.j 0.+0.j 1.+0.j 0.+0.j]
```

Type
ndarray or int

property beta

1 qubit state of the central spin in S_z basis

OR index of the energy state to be considered as one.

Type
ndarray or int

property state

Initial state of the qubit in gCCE simulations. Assumed to be $\frac{1}{\sqrt{2}}(0+1)$ unless provided.

Type
ndarray

property gyro

Tensor describing central spin interactions with the magnetic field or array of spins.

Default -17608.597050 rad / ms / G - gyromagnetic ratio of the free electron spin.

Type
ndarray with shape (3,3) or (n, 3, 3)

add_single_jump(*operator*, *rate=1*, *units='rad'*, *square_root=False*, *which=None*)

Add single-spin jump operator for the spin to be used in the Lindbladian master equation CCE.

Parameters

- **operator** (*str or ndarray with shape (dim, dim)*) – Definition of the operator. Can be either of the following: * Pair of integers defining the Sven operator. * String where each symbol corresponds to the spin matrix or operation between them.

  Allowed symbols: `xyz+`. If there is nothing between symbols, assume multiplication of the operators. If there is a + symbol, assume summation between terms. For example, `xx+z` would correspond to the operator $\hat{S}_x\hat{S}_x + \hat{S}_z$.

  - String equal to `A`. Then assumes that the correct matrix form of the operator has been provided by the user.

- **rate** (*float*) – Rate associated with the given jump operator. By default, is given in rad ms^-1.
- **units** (*str*) – Units of the rate, can be either rad (for radial frequency units) or deg (for rotational frequency).
- **square_root** (*bool*) – True if the rate is given as a square root of the rate (to match how one sets up collapse operators in Qutip). Default False.
- **which** (*int*) – For which central spin in the center array add the jump operator. Default is None - if there is only one central spin then the jump operator is added, otherwise the exception is raised.

set_zfs(*D=0*, *E=0*)

Set Zero Field Splitting of the central spin from longitudinal ZFS *D* and transverse ZFS *E*.

Parameters

- **D** (*float or ndarray with shape (3, 3)*) – D (longitudinal splitting) parameter of central spin in ZFS tensor of central spin in kHz.

  OR

  Total ZFS tensor. Default 0.

- **E** (*float*) – E (transverse splitting) parameter of central spin in ZFS tensor of central spin in kHz. Default 0. Ignored if `D` is None or tensor.

set_gyro(*gyro*)

Set gyromagnetic ratio of the central spin.

Parameters

gyro (*float or ndarray with shape (3, 3)*) – Gyromagnetic ratio of central spin in rad / ms / G.

OR

Tensor describing central spin interactions with the magnetic field.

Default -17608.597050 kHz * rad / G - gyromagnetic ratio of the free electron spin.

point_dipole()

Using point-dipole approximation, generate interaction tensors between central spins.

generate_states(*magnetic_field=None*, *bath=None*, *projected_bath_state=None*)

Compute eigenstates of the central spin Hamiltonian.

Parameters

- **magnetic_field** (*ndarray with shape (3,)*) – Array containing external magnetic field as (Bx, By, Bz).
- **bath** (*BathArray with shape (m,) or ndarray with shape (m, 3, 3)* – Array of all bath spins or array of hyperfine tensors.
- **projected_bath_state** (*ndarray with shape (m,) or (m, 3)*) – Array of I_z projections for each bath spin.

generate_projections(*second_order=False*, *level_confidence=0.95*)

Generate vectors with the spin projections of the spin states:

$$[a\hat{S}_x a, a\hat{S}_y a, a\hat{S}_z a],$$

where a and is alpha or beta qubit state. They are stored in the `.projections_alpha` and `.projections_beta` respectively.

If `second_order` is set to `True`, also generates matrix elements of qubit states and all other eigenstates of the central spin Hamiltonian, used in computing second order couplings between bath spins:

$$[a\hat{S}_x b, a\hat{S}_y b, a\hat{S}_z b],$$

where a is qubit level and b are all other energy levels.

This function is called in the `CCE` routine.

Note: if qubit state are not eigenstates and `second_order` set to `True`, for each qubit state finds a close eigenstate (with minimal fidelity between two states set by `level_confidence` keyword) and uses that one instead of user provided.

Parameters

- **second_order** (*bool*) – True if generate properties, necessary for second order corrections.
- **level_confidence** (*float*) – Minimum fidelity between an eigenstate and provided qubit level for them to be considered the same. Used only if `second_order == True`.

`get_energy`(*which*)

Get energy of the qubit state.

Parameters
which (*str*) – `alpha` for 0 qubit state, `beta` for 1 qubit state.

Returns
Energy of the qubit state.

Return type
float

`generate_sigma`()

Generate Pauli matrices of the qubit in S_z basis.

`add_interaction`(*i*, *j*, *tensor*)

Add interactions tensor between bath spins with indexes `i` and `j`.

Parameters

- **i** (*int or ndarray (n,)*) – Index of the first spin in the pair or array of the indexes of the first spins in n pairs.
- **j** (*int or ndarray with shape (n,)*) – Index of the second spin in the pair or array of the indexes of the second spins in n pairs.
- **tensor** (*ndarray with shape (3,3) or (n, 3,3)*) – Interaction tensor between the spins i and j or array of tensors.

5.2 Center

Documentation for the `pycce.Center` class - inner class, containing properties of a single central spin.

`class Center`(*position=None*, *spin=0*, *D=0*, *E=0*, *gyro=-17608.59705*, *alpha=None*, *beta=None*, *detuning=0*)

Class, which contains the properties of the single central spin. Should *not* be initialized directly - use `CenterArray` instead.

Parameters

- **position** (*ndarray with shape (3,)*) – Cartesian coordinates in Angstrom of the central spin. Default (0., 0., 0.).
- **spin** (*float*) – Total spin of the central spin.
- **D** (*float or ndarray with shape (3,)*) – D (longitudinal splitting) parameter of central spin in ZFS tensor of central spin in kHz.

  OR

  Total ZFS tensor. Default 0.
- **E** (*float*) – E (transverse splitting) parameter of central spin in ZFS tensor of central spin in kHz. Default 0. Ignored if `D` is None or tensor.
- **gyro** (*float or ndarray with shape (3, 3)*) – Gyromagnetic ratio of central spin in rad / ms / G.

  OR

  Tensor describing central spin interactions with the magnetic field.

  Default -17608.597050 kHz * rad / G - gyromagnetic ratio of the free electron spin.

- **alpha** (*int or ndarray with shape (2*spin + 1,)*) – 0 state of the qubit in S_z basis or the index of eigenstate to be used as one.

  Default is **None**.

- **beta** (*int or ndarray with shape (2*spin + 1,)*) – 1 state of the qubit in S_z basis or the index of eigenstate to be used as one.

  Default is **None**.

- **detuning** (*float*) – Energy detuning from the zeeman splitting in kHz, included as an extra $+\omega\hat{S}_z$ term in the Hamiltonian, where ω is the detuning.

  Default 0.

projections_alpha

Vector with spin operator matrix elements of type $[0\hat{S}_x0, 0\hat{S}_y0, 0\hat{S}_z0]$, where 0 is the alpha qubit state. Generated by `CenterArray`.

Type
ndarray with shape (3,)

projections_beta

Vector with spin operator matrix elements of type $[1\hat{S}_x1, 1\hat{S}_y1, 1\hat{S}_z1]$, where 1 is the beta qubit state. Generated by `CenterArray`.

Type
ndarray with shape (3,)

projections_alpha_all

ndarray with shape (2s-1, 3): Array of vectors of the central spin matrix elements of form:

$$[0\hat{S}_xj, 0\hat{S}_yj, 0\hat{S}_zj],$$

where 0 is the alpha qubit state, and æ are all states.

projections_beta_all

ndarray with shape (2s-1, 3): Array of vectors of the central spin matrix elements of form:

$$[1\hat{S}_xj, 1\hat{S}_yj, 1\hat{S}_zj],$$

where 1 is the beta qubit state, and æ are all states.

energies

Array of the central spin Hamiltonian eigen energies.

Type
ndarray with shape (2s-1,)

eigenvectors

Eigen states of the central spin Hamiltonian.

Type
ndarray

hamiltonian

Central spin Hamiltonian.

Type
Hamiltonian

`alpha_index`

Index of the central spin Hamiltonian eigen state, chosen as alpha state of the qubit.

Type
int

`beta_index`

Index of the central spin Hamiltonian eigen state, chosen as beta state of the qubit.

Type
int

`property xyz`

Position of the central spin in Cartesian coordinates.

Type
ndarray with shape (3,)

`property gyro`

Tensor describing central spin interactions with the magnetic field or array of spins.

Default -17608.597050 rad / ms / G - gyromagnetic ratio of the free electron spin.

Type
ndarray with shape (3,3) or (n, 3, 3)

`property zfs`

Zero field splitting tensor of the central spin or array of spins.

Type
ndarray with shape (3, 3) or (n, 3, 3)

`property s`

Total spin of the central spin or array of spins.

Type
float or ndarray with shape (n,)

`property h`

Dictionary with additional spin Hamiltonian parameters. Key denotes the product of spin operators as:

Either a string containing `x, y, z, +, -` where each symbol is a corresponding spin operator:

- `x` == S_x
- `y` == S_y
- `z` == S_z
- `p` == S_+
- `m` == S_-

Several symbols is a product of those spin operators.

Or a tuple with indexes (k, q) for Stevens operators (see https://www.easyspin.org/documentation/stevensoperators.html).

The item is the coupling parameter in float.

Examples

- `d['pm'] = 2000` corresponds to the Hamiltonian term $\hat{H}_{add} = A\hat{S}_+\hat{S}_-$ with $A = 2$ MHz.
- `d[2, 0] = 1.5e6` corresponds to Stevens operator $B_k^q\hat{O}_k^q = 3\hat{S}_z - s(s+1)\hat{I}$ with $k = 2$, $q = 0$, and $B_k^q = 1.5$ GHz.

Type
dict

property detuning

Position of the central spin in Cartesian coordinates.

Type
ndarray with shape (3,)

add_single_jump(*operator*, *rate=1*, *units='rad'*, *square_root=False*, *which=None*)

Add single-spin jump operator for the spin to be used in the Lindbladian master equation CCE.

Parameters

- **operator** (*str or ndarray with shape (dim, dim)*) – Definition of the operator. Can be either of the following: * Pair of integers defining the Sven operator. * String where each symbol corresponds to the spin matrix or operation between them.

  Allowed symbols: `xyz+`. If there is nothing between symbols, assume multiplication of the operators. If there is a + symbol, assume summation between terms. For example, `xx+z` would correspond to the operator $\hat{S}_x\hat{S}_x + \hat{S}_z$.

  – String equal to `A`. Then assumes that the correct matrix form of the operator has been provided by the user.

- **rate** (*float*) – Rate associated with the given jump operator. By default, is given in rad ms^-1.
- **units** (*str*) – Units of the rate, can be either rad (for radial frequency units) or deg (for rotational frequency).
- **square_root** (*bool*) – True if the rate is given as a square root of the rate (to match how one sets up collapse operators in Qutip). Default False.
- **which** (*int*) – For which central spin in the center array add the jump operator. Default is None - if there is only one central spin then the jump operator is added, otherwise the exception is raised.

set_zfs(*D=0*, *E=0*)

Set Zero Field Splitting of the central spin from longitudinal ZFS *D* and transverse ZFS *E*.

Parameters

- **D** (*float or ndarray with shape (3, 3)*) – D (longitudinal splitting) parameter of central spin in ZFS tensor of central spin in kHz.

  OR

  Total ZFS tensor. Default 0.

- **E** (*float*) – E (transverse splitting) parameter of central spin in ZFS tensor of central spin in kHz. Default 0. Ignored if `D` is None or tensor.

set_gyro(*gyro*)

Set gyromagnetic ratio of the central spin.

Parameters

gyro (*float or ndarray with shape (3, 3)*) – Gyromagnetic ratio of central spin in rad / ms / G.

OR

Tensor describing central spin interactions with the magnetic field.

Default -17608.597050 kHz * rad / G - gyromagnetic ratio of the free electron spin.

property alpha

0 qubit state of the central spin in S_z basis

OR

index of the energy state to be considered as one.

Type

ndarray or int

property beta

1 qubit state of the central spin in S_z basis

OR

index of the energy state to be considered as one.

Type

ndarray or int

property dim

Dimensions of the central spin or array of spins.

Type

int or ndarray with shape (n,)

generate_sigma()

Generate Pauli matrices of the qubit in S_z basis.

property sigma

Dictionary with Pauli matrices of the qubit in S_z basis.

Type

dict

generate_states(*magnetic_field=None*, *bath=None*, *projected_bath_state=None*)

Compute eigenstates of the central spin Hamiltonian.

Parameters

- **magnetic_field** (*ndarray with shape (3,)*) – Array containing external magnetic field as (Bx, By, Bz).
- **bath** (*BathArray with shape (m,) or ndarray with shape (m, 3, 3*) – Array of all bath spins or array of hyperfine tensors.
- **projected_bath_state** (*ndarray with shape (m,) or (m, 3)*) – Array of I_z projections for each bath spin.

generate_hamiltonian(*magnetic_field=None*, *bath=None*, *projected_bath_state=None*)

Generate central spin Hamiltonian.

Parameters

- **magnetic_field** (*ndarray with shape (3,) or func*) – Magnetic field of type `magnetic_field = np.array([Bx, By, Bz])` or callable with signature `magnetic_field(pos)`, where `pos` is ndarray with shape (3,) with the position of the spin.
- **bath** (*BathArray with shape (n,) or ndarray with shape (n, 3, 3)*) – Array of bath spins or hyperfine tensors.
- **projected_bath_state** (*ndarray with shape (n,)*) – S_z projections of the bath spin states.

Returns

Central spin Hamiltonian, including
first order contributions from the bath spins.

Return type
Hamiltonian

transform(*rotation=None*, *style='col'*)

Apply coordinate transformation to the central spin.

Parameters

- **rotation** (*ndarray with shape (3, 3)*) – Rotation matrix.
- **style** (*str*) – Can be 'row' or 'col'. Determines how rotation matrix is initialized.

CHAPTER

SIX

RUNNING THE SIMULATIONS

6.1 Setting up the Simulator Object

Documentation for the `pycce.Simulator` - main class for conducting CCE Simulations.

class Simulator(*spin*, *position=None*, *alpha=None*, *beta=None*, *gyro=None*, *magnetic_field=None*, *D=None*, *E=0.0*, *r_dipole=None*, *order=None*, *bath=None*, *pulses=None*, *as_delay=False*, *n_clusters=None*, ***bath_kw*)

The main class for CCE calculations.

The typical usage includes:

1. Read array of the bath spins. This is done with `Simulator.read_bath` method which accepts either reading from .xyz file or from the `BathArray` instance with defined positions and names of the bath spins. In the process, the subset of the array within the distance of `r_dipole` from the central spin is taken and for this subset the Hyperfine couplings can be generated.

   If no `hyperfine` keyword is provided and there are some hyperfine couplings already, then no changes are done to the hyperfine tensors. If `hyperfine='pd'`, the hyperfine couplings are computed assuming point dipole approximation. For all accepted arguments, see `Simulator.read_bath`.

2. Generate set of clusters with `Simulator.generate_clusters`, determined by the maximum connectivity radius `r_dipole` and the maximum size of the cluster `order`.

3. Compute the desired property with `Simulator.compute` method.

Note: Directly setting up the attribute values will rerun `Simulator.read_bath` and/or `Simulator.generate_clusters` to reflect updated value of the given attribute.

E.g. If `Simulator.r_bath` is set to some new value after initialization, then `Simulator.read_bath` and `Simulator.generate_clusters` are called with the increased bath.

First two steps are usually done during the initialization of the `Simulator` object by providing the necessary arguments.

Notes

Depending on the number of provided arguments, in the initialization process will call the following methods to setup the calculation engine.

- If `bath` is provided, `Simulator.read_bath` is called with additional keywords in `**bath_kw`.
- If both `r_dipole` and `order` are provided and `bath` is not None, the `Simulator.generate_clusters` is called.

See the corresponding method documentation for details.

Examples:

```
>>> atoms = random_bath('13C', 100, number=2000, seed=10)
>>> calc = Simulator(1, bath=atoms, r_bath=40, r_dipole=6,
>>>                  order=2, D=2.88 * 1e6,
>>>                  magnetic_field=500, pulses=1)
>>> print(calc)
Simulator for center array of size 1.
Parameters of cluster expansion:
r_bath: 40
r_dipole: 6
order: 2

Bath consists of 549 spins.

Clusters include:
549  clusters of order 1.
457  clusters of order 2.
```

Parameters

- **spin** (*CenterArray or float or array with shape (n,)*) – CenterArray containing properties of all central spins.

  OR

  Total spin of the central spin (Assumes one central spin).

  OR

  Array of total spins of the central spins (Assumes *n* central spins).

- **position** (*ndarray*) – Cartesian coordinates ar array of coordinates in Angstrom of the central spin(s). Default (0., 0., 0.). If provided, overrides the position in CenterArray.

- **alpha** (*float or ndarray with shape (S,)*) – 0 state of the qubit in S_z basis or the index of eigenstate to be used as one.

  Default: Lowest energy eigenstate of the central spin Hamiltonian.

  If provided, overrides the alpha state in the CenterArray.

- **beta** (*float or ndarray with shape (S,)*) – 1 state of the qubit in S_z basis or the index of the eigenstate to be used as one.

  Default: Second lowest energy eigenstate of the central spin Hamiltonian.

  If provided, overrides the beta state in the CenterArray.

- **gyro** (*float or ndarray with shape (3, 3)*) – Gyromagnetic ratio of the central spin(s) in rad / ms / G.

  OR

  Tensor describing central spin interactions with the magnetic field.

  Default -17608.597050 kHz * rad / G - gyromagnetic ratio of the free electron spin.

  If provided, overrides the gyro value in CenterArray.

- **D** (*float or ndarray with shape (3, 3)*) – D (longitudinal splitting) parameter of central spin in ZFS tensor of central spin in kHz.

  OR

  Total ZFS tensor. Default 0.

  If provided, overrides the ZFS value in CenterArray.

- **E** (*float*) – E (transverse splitting) parameter of central spin in ZFS tensor of central spin in kHz. Default 0. Ignored if `D` is None or tensor.

- **bath** (*ndarray or str*) – First positional argument of the `Simulator.read_bath` method.

  Either:

  - Instance of BathArray class;
  - ndarray with `dtype([('N', np.unicode_, 16), ('xyz', np.float64, (3, ))])` containing names of bath spins (same ones as stored in self.ntype) and positions of the spins in angstroms;
  - the name of the .xyz text file containing 4 columns: name of the bath spin and xyz coordinates in A.

- **r_dipole** (*float*) – Maximum connectivity distance between two bath spins.

- **order** (*int*) – Maximum size of the cluster to be considered in CCE expansion.

- **n_clusters** (*dict*) – Dictionary which contain maximum number of clusters of the given size. Has the form `n_clusters = {order: number}`, where `order` is the size of the cluster, `number` is the maximum number of clusters with this size.

  If provided, sort the clusters by the "strength" of cluster. Then the strongest `number` of clusters is taken.

  We define the strength of the cluster s as an inverse of the sum over inverse pairwise interaction strengths of the minimal cluster:

  $$s = (\sum_{i<j\in C} \frac{r^3}{\gamma_i \gamma_j})^{-1}$$

  Where γ_i is the gyromagnetic ration of a spin i, r is the distance between two spins, and the summation of i, j goes only over the edges of the minimally connected cluster.

  We define minimally connected cluster as a cluster with lowest possible number of edges that still forms a connected graph. If multiple choices of the minimally connected cluster for the same cluster are possible, the one with the larger strength s is chosen.

- **pulses** (*list or int or* `Sequence`) – Number of pulses in CPMG sequence or list with pulses.

- ****bath_kw** – Additional keyword arguments for the `Simulator.read_bath` method.

`center`

Array of central spins.

Type
CenterArray

`clusters`

Dictionary containing information about cluster structure of the bath.

Each keys n correspond to the size of the cluster. Each `Simulator.clusters[n]` contains `ndarray` of shape (m, n), where m is the number of clusters of given size, n is the size of the cluster. Each row of this array contains indexes of the bath spins included in the given cluster. Generated during `.generate_clusters` call.

Type
dict

`as_delay`

True if time points are delay between pulses (for equispaced pulses), False if time points are total time. Ignored if `pulses` contains the time delays.

Type
bool

`interlaced`

True if use hybrid CCE approach - for each cluster sample over states of the supercluster.

Type
bool

`seed`

Seed for random number generator, used in random bath states sampling.

Type
int

`nbstates`

Number or random bath states to sample over.

Type
int

`fixstates`

If not None, shows which bath states to fix in random bath states.

Each key is the index of bath spin, value - fixed $\hat{S}_z$ projection of the mixed state of nuclear spin.

Type
dict

`masked`

True if mask numerically unstable points (with coherence > 1) in the averaging over bath states.

Note: It is up to user to check whether the possible instability is due to numerical error or unphysical assumptions of the calculations.

Type
bool

`second_order`

True if add second order perturbation theory correction to the cluster Hamiltonian in conventional CCE. Relevant only for conventional CCE calculations.

Type
bool

`level_confidence`

Maximum fidelity of the qubit state to be considered eigenstate of the central spin Hamiltonian when `second_order` set to True.

Type
float

`projected_bath_state`

Array with z-projections of the bath spins states.

Type
ndarray with shape (n,)

`bath_state`

Array of bath states.

Type
bath_state (ndarray)

`timespace`

Time points at which compute the desired property.

Type
timespace (ndarray with shape (n,))

`property alpha`

0 qubit state of the central spin in Sz basis **OR** index of the energy state to be considered as one.

Type
ndarray or int

Type
Returns .center.alpha property

`property beta`

1 qubit state of the central spin in Sz basis **OR** index of the energy state to be considered as one.

Type
ndarray or int

Type
Returns .center.beta property

`property magnetic_field`

Array containing external magnetic field as (Bx, By, Bz) or callable with signature `magnetic_field(pos)`, where `pos` is an array with shape (3,) with the position of either bath or central spin. Default is (0, 0, 0).

Type
ndarray

`property order`

Maximum size of the cluster.

Type
int

property n_clusters

Dictionary which contain maximum number of clusters of the given size. Has the form `n_clusters = {order: number}`, where `order` is the size of the cluster, `number` is the maximum number of clusters with this size.

If provided, sorts the clusters by the strength of cluster interaction, equal to the inverse of a sum of inverse pairwise interaction in the minimally connected cluster. Then the strongest `number` of clusters is taken.

Type
dict

property r_dipole

Maximum connectivity distance.

Type
float

property pulses

List-like object, containing the sequence of the instantaneous ideal control pulses.

Each item is `Pulse` object, containing the following attributes:

- **which** (*array-like*): Indexes of the central spins to be rotated by the pulse. Default is all.
- **x** (*float*): Rotation angle of the central spin about x-axis in radians.
- **y** (*float*): Rotation angle of the central spin about y-axis in radians.
- **z** (*float*): Rotation angle of the central spin about z-axis in radians.
- **delay** (*float or ndarray*): Delay before the pulse or array of delays with the same shape as time points.

Additionally, act as a container object for the pulses, applied to the bath.

The bath pulses can be accessed as items of the `Pulse` object, with name of the item corresponding to the name of the bath spin impacted, and the item corresponding to the `BasePulse` object with attributes:

- **x** (*float*): Rotation angle of the central spin about x-axis in radians.
- **y** (*float*): Rotation angle of the central spin about y-axis in radians.
- **z** (*float*): Rotation angle of the central spin about z-axis in radians.

Examples

```
>>> p = Pulse('x', 'pi')
>>> print(p)
Pulse((x: 3.14, y: 0.00, z: 0.00))
>>> pb = Pulse('x', 'pi', bath_names=['13C', '14C'])
>>> print(pb)
Pulse((x: 3.14, y: 0.00, z: 0.00), {13C: (x: 3.14, y: 0.00, z: 0.00),
                                    14C: (x: 3.14, y: 0.00, z: 0.00)})
>>> print(pb['13C'])
(x: 3.14, y: 0.00, z: 0.00)
```

If delay is not provided in **all** pulses, assumes even delay of CPMG sequence. If only **some** delays are provided, assumes 0 delay in the pulses without delay provided.

For the full list of properties, see `Pulse` and `Sequence` documentations.

Type
Sequence

property r_bath

Cutoff size of the spin bath. If `len(r_bath) > 1`, uses different cutoff sizes for each of the central spins. The total bath then is the sum of all bath spins, that are close to at least one of the central spins.

Type
float or array-like

property external_bath

Array with spins read from DFT output (see `pycce.io`).

Type
BathArray

property ext_r_bath

Maximum distance from the central spins of the bath spins for which to use the data from `external_bath`.

Type
float

property error_range

Maximum distance between positions in bath and external bath to consider two positions the same (default 0.2).

Type
float

property hyperfine

This argument tells the code how to generate hyperfine couplings. If (`hyperfine = None` and all A in provided bath are 0) or (`hyperfine = 'pd'`), use point dipole approximation. Otherwise can be an instance of `Cube` object, or callable with signature:

```
func(array)
```

where array is the `BathArray` object.

Type
str, func, or Cube instance

property bath

Array of bath spins used in CCE simulations.

Type
BathArray

set_zfs(*D=None*, *E=0*)

Set Zero Field Splitting of the central spin from longitudinal ZFS *D* and transverse ZFS *E*.

Parameters

- **D** (*float or ndarray with shape (3, 3)*) – D (longitudinal splitting) parameter of central spin in ZFS tensor of central spin in kHz.

  OR

  Total ZFS tensor. Default 0.

- **E** (*float*) – E (transverse splitting) parameter of central spin in ZFS tensor of central spin in kHz. Default 0. Ignored if `D` is None or tensor.

set_magnetic_field(*magnetic_field=None*)

Set magnetic field from either value of the magnetic field along z-direction or full magnetic field vector.

Parameters

magnetic_field (*float or array-like*) – Magnetic field along z-axis.

OR

Array containing external magnetic field as (Bx, By, Bz). Default (0, 0, 0).

6.2 Reading the Bath

Documentation for the `Simulator.read_bath` and `Simulator.generate_clusters` method. These methods are called automatically on the initialization of the `Simulator` object if the necessary keywords are provided. Otherwise they can also be called by themselves to update the properties of the spin bath in `Simulator` object.

`Simulator.`**read_bath**(*bath=None*, *r_bath=None*, *skiprows=1*, *external_bath=None*, *hyperfine=None*, *types=None*, *error_range=None*, *ext_r_bath=None*, *imap=None*, *func_kw=None*)

Read spin bath from the file or from the `BathArray`.

Parameters

- **bath** (*ndarray, BathArray or str*) – Either:
  - Instance of BathArray class;
  - ndarray with `dtype([('N', np.unicode_, 16), ('xyz', np.float64, (3, ))])` containing names of bath spins (same ones as stored in self.ntype) and positions of the spins in angstroms;
  - the name of the xyz text file containing 4 cols: name of the bath spin and xyz coordinates in A.
- **r_bath** (*float or array-like*) – Cutoff size of the spin bath. If `len(r_bath) > 1`, uses different cutoff sizes for each of the central spins. The total bath then is the sum of all bath spins, that are close to at least one of the central spins.
- **skiprows** (*int, optional*) – If `bath` is name of the file, this argument gives number of rows to skip while reading the .xyz file (default 1).
- **external_bath** (*BathArray, optional*) – BathArray containing spins read from DFT output (see `pycce.io`).
- **hyperfine** (*str, func, or Cube instance, optional*) – This argument tells the code how to generate hyperfine couplings.

  If (`hyperfine = None` and all A in provided bath are 0) or (`hyperfine = 'pd'`), use point dipole approximation.

  Otherwise can be an instance of `Cube` object, or callable with signature:

  ```
  func(array, *args, **kwargs)
  ```

  where `array` is array of the bath spins,
- **func_kw** (*dict*) – Additional keywords if for generating hyperfine couplings if `hyperfine` is callable.
- **types** (*SpinDict*) – SpinDict or input to create one. Contains either SpinTypes of the bath spins or tuples which will initialize those.

See `pycce.bath.SpinDict` documentation for details.

- **error_range** (*float, optional*) – Maximum distance between positions in bath and external bath to consider two positions the same (default 0.2).
- **ext_r_bath** (*float, optional*) – Maximum distance from the central spins of the bath spins for which to use the DFT positions.
- **imap** (InteractionMap) – Instance of `InteractionMap` class, containing interaction tensors for bath spins. Each key of the `InteractionMap` is a tuple with indexes of two bath spins. The value is the 3x3 tensor describing the interaction between two spins in a format:

$$I^i J I^j = I^i_x J_{xx} I^j_x + I^i_x J_{xy} I^j_y ...$$

Note: For each bath spin pair without interaction tensor in `imap`, coupling is approximated assuming magnetic point dipole–dipole interaction. If `imap = None` all interactions between bath spins are approximated in this way. Then interaction tensor between spins *i* and *j* is computed as:

$$\mathbf{J}_{ij} = -\gamma_i \gamma_j \frac{\hbar^2}{4\pi\mu_0} \left[\frac{3\vec{r}_{ij} \otimes \vec{r}_{ij} - |r_{ij}|^2 I}{|r_{ij}|^5} \right]$$

Where γ_i is gyromagnetic ratio of *i* spin, I is 3x3 identity matrix, and $\vec{r}_{ij}$ is distance between two spins.

Returns
The view of `Simulator.bath` attribute, generated by the method.

Return type
BathArray

`Simulator.`**generate_clusters**(*order=None*, *r_dipole=None*, *r_inner=0*, *strong=False*, *ignore=None*, *n_clusters=None*)

Generate set of clusters used in CCE calculations.

The clusters are generated from the following procedure:

- Each bath spin i forms a cluster of one.
- Bath spins i and j form cluster of two if there is an edge between them (distance $d_{ij} \leq$ `r_dipole`).
- Bath spins i, j, and j form a cluster of three if enough edges connect them (e.g., there are two edges ij and jk)
- And so on.

In general, we assume that spins $\{i..n\}$ form clusters if they form a connected graph. Only clusters up to the size imposed by the `order` parameter (equal to CCE order) are included.

Parameters

- **order** (*int*) – Maximum size of the cluster.
- **r_dipole** (*float*) – Maximum connectivity distance.
- **r_inner** (*float*) – Minimum connectivity distance.
- **strong** (*bool*) – True - generate only clusters with "strong" connectivity (all nodes should be interconnected). Default False.
- **ignore** (*list or str, optional*) – If not None, includes the names of bath spins which are ignored in the cluster generation.

- **n_clusters** (*dict*) – Dictionary which contain maximum number of clusters of the given size. Has the form `n_clusters = {order: number}`, where `order` is the size of the cluster, `number` is the maximum number of clusters with this size.

  If provided, sort the clusters by the strength of cluster interaction, Then the strongest `number` of clusters is taken.

  Strength of the cluster s is defined as an inverse of a sum of inverse pairwise interactions of the minimal cluster:

$$s = (\sum_{i<j \in C} \frac{r^3}{\gamma_i \gamma_j})^{-1}$$

Returns

View of `Simulator.clusters`. `Simulator.clusters` is a dictionary
with keys corresponding to size of the cluster.

I.e. `Simulator.clusters[n]` contains `ndarray` of shape (m, n), where m is the number of clusters of given size, n is the size of the cluster. Each row contains indexes of the bath spins included in the given cluster.

Return type
dict

6.3 Calculate Properties with Simulator

Documentation for the `Simulator.compute` method - the interface to run calculations with **PyCCE**.

`Simulator.`**`compute`**(*timespace*, *quantity='coherence'*, *method='cce'*, ***kwargs*)

General function for computing properties with CCE.

The dynamics are simulated using the Hamiltonian:

$$\hat{H}_S = \mathbf{SDS} + \mathbf{B}\gamma_S\mathbf{S}$$
$$\hat{H}_{SB} = \sum_i \mathbf{S}\mathbf{A}_i\mathbf{I}_i$$
$$\hat{H}_B = \sum_i \mathbf{I}_i\mathbf{P}_i\mathbf{I}_i + \mathbf{B}\gamma_i\mathbf{I}_i + \sum_{i>j} \mathbf{I}_i\mathbf{J}_{ij}\mathbf{I}_j$$

Here $\hat{H}_S$ is the central spin Hamiltonian with Zero Field splitting tensor $\mathbf{D}$ and gyromagnetic ratio tensor $\gamma_\mathbf{S} = \mu_S\mathbf{g}$ are read from `Simulator.zfs` and `Simulator.gyro` respectively.

The $\hat{H}_{SB}$ is the Hamiltonian describing interactions between central spin and the bath. The hyperfine coupling tensors $\mathbf{A}_i$ are read from the `BathArray` stored in `Simulator.bath['A']`. They can be generated using point dipole approximation or provided by the user (see `Simulator.read_bath` for details).

The $\hat{H}_B$ is the Hamiltonian describing interactions between the bath spins. The self interaction tensors $\mathbf{P}_i$ are read from the `BathArray` stored in `Simulator.bath['Q']` and have to be provided by the user.

The gyromagnetic ratios γ_i are read from the `BathArray.gyros` attribuite, which is generated from the properties of the types of bath spins, stored in `BathArray.types`. They can either be provided by user or read from the `pycce.common_isotopes` object.

The interaction tensors $\mathbf{J}_{ij}$ are assumed from point dipole approximation or can be provided in `BathArray.imap` attrubite.

Note: The `compute` method takes two keyword arguments to determine which quantity to compute and how:

- *method* can take 'cce' or 'gcce' values, and determines which method to use - conventional or generalized CCE.
- *quantity* can take 'coherence' or 'noise' values, and determines which quantity to compute - coherence function or autocorrelation function of the noise.

Each of the methods can be performed with monte carlo bath state sampling (if `nbstates` keyword is non zero) and with interlaced averaging (If `interlaced` keyword is set to `True`).

Examples

First set up Simulator object using random bath of 1000 13C nuclear spins.

```
>>> import pycce as pc
>>> import numpy as np
>>> atoms = pc.random_bath('13C', 100, number=2000, seed=10) # Random spin bath
>>> calc = pc.Simulator(1, bath=atoms, r_bath=40, r_dipole=6,
>>>                     order=2, D=2.88 * 1e6, # D of NV in GHz -> kHz
>>>                     magnetic_field=500, pulses=1)
>>> ts = np.linspace(0, 2, 101) # timesteps
```

We set magnetic field to 500 G along z-axis and chose 1 decoupling pulse (Hahn-echo) in this example. The zero field splitting is set to the one of NV center in diamond.

Run conventional CCE calculation at time points `timespace` to obtain coherence without second order effects:

```
>>> calc.compute(ts)
```

This will call `Simulator.cce_coherence` method with default keyword values.

Compute the coherence conventional CCE coherence with second order interactions between bath spins:

```
>>> calc.compute(ts, second_order=True)
```

Compute the coherence with conventional CCE with bath state sampling (over 10 states):

```
>>> calc.compute(ts, nbstates=10)
```

Compute the coherence with generalized CCE:

```
>>> calc.compute(ts, method='gcce')
```

This will call `Simulator.gcce_dm` method with default keyword values and obtain off diagonal element as $0\hat{\rho}_C 1$, where $\hat{\rho}_C$ is the density matrix of the qubit.

Compute the coherence with generalized CCE with bath state sampling (over 10 states):

```
>>> calc.compute(ts, method='gcce', nbstates=10)
```

Parameters

- **timespace** (*ndarray with shape (n,)*) – Time points at which compute the desired property.

- **quantity** (*str*) – Which quantity to compute. Case insensitive.

  Possible values:

  – 'coherence': compute coherence function.

  – 'noise': compute noise autocorrelation function.

- **method** (*str*) – Which implementation of CCE to use. Case insensitive.

  Possible values:

  – 'cce': conventional CCE, where interactions are mapped on 2 level pseudospin.

  – 'gcce': Generalized CCE where central spin is included in each cluster.

- **magnetic_field** (*ndarray with shape (3,) or callable*) – Magnetic field vector of form (Bx, By, Bz) or callable with signature `magnetic_field(pos)`, where `pos` is an array with shape (3,) with the position of the spin.

  Default is **None**. Overrides `Simulator.magnetic_field` if provided.

- **pulses** (*list or int or* Sequence) – Number of pulses in CPMG sequence.

  OR

  Sequence of the instantaneous ideal control pulses. It can be provided as an instance of `Sequence` class or a list with `Pulse` objects. (See documentation for pycce.Sequence).

  `pulses` can be provided as a list with tuples or dictionaries, each tuple or dictionary is used to initialize `Pulse` class instance.

  For example, for only central spin pulses the `pulses` argument can be provided as a list of tuples, containing:

  1. axis the rotation is about;
  2. angle of rotation;
  3. (optional) Time before the pulse. Can be as fixed, as well as varied. If varied, it should be provided as an array with the same length as `timespace`.

  E.g. for Hahn-Echo the `pulses` can be defined as `[('x', np.pi)]` or `[('x', np.pi, timespace / 2)]`.

  Note: If delay is not provided in **all** pulses, assumes even delay of CPMG sequence. If only **some** delays are provided, assumes `delay = 0` in the pulses without delay.

  Then total experiment is assumed to be:

  tau – pulse – 2tau – pulse – … – 2tau – pulse – tau

  Where tau is the delay between pulses.

  The sum of delays at each time point should be less or equal to the total time of the experiment at the same time point, provided in `timespace` argument.

  Warning: In conventional CCE calculations, only pi pulses on the central spin are allowed.

  In the calculations of noise autocorrelation this parameter is ignored.

  Default is **None**. Overrides``Simulator.pulses`` if provided.

- **i** (*int or ndarray with shape (2s+1,) or callable*) – Used in gCCE calculations. Along with `j` parameter indicates which density matrix element to compute with gCCE as:

$$L = i\hat{\rho}j$$

  By default is equal to $R0$ state of the `.center` where R is a product of all rotations applied in the pulse sequence. Can be set as a vector in S_z basis, the index of the central spin Hamiltonian eigenstate, or as a callable with call signature `i(dm)`, where `dm` is a density matrix of the central spin. If callable, `j` parameter is ignored.

- **j** (*int or ndarray with shape (2s+1,) or callable*) – Used in gCCE calculations. Along with `i` parameter indicates which density matrix element to compute.

  By default is equal to $R1$ state of the `.center` where R is a product of all rotations applied in the pulse sequence. Can be set as a vector in S_z basis, the index of the central spin Hamiltonian eigenstate, or as a callable with call signature `j(dm)`, where `dm` is a density matrix of the central spin. If callable, `i` parameter is ignored.

- **as_delay** (*bool*) – True if time points are delay between pulses (for equispaced pulses), False if time points are total time. Ignored in gCCE if `pulses` contains the time fractions. Conventional CCE calculations do not support custom time fractions.

  Default is **False**.

- **interlaced** (*bool*) – True if use hybrid CCE approach - for each cluster sample over states of the supercluster.

  Default is **False**.

- **state** (*ndarray with shape (2s+1,)*) – Initial state of the central spin, used in gCCE and noise autocorrelation calculations.

  Defaults to $\frac{1}{N}(0+1)$ if not set.

- **bath_state** (*array-like*) – List of bath spin states. If `len(shape) == 1`, contains I_z projections of I_z eigenstates. Otherwise, contains array of initial density matrices of bath spins.

  Default is **None**. If not set, the code assumes completely random spin bath (density matrix of each nuclear spin is proportional to identity, $\hat{\mathbb{1}}/N$).

- **nbstates** (*int*) – Number or random bath states to sample over.

  If provided, sampling of random states is carried and `bath_states` values are ignored.

  Default is 0.

- **seed** (*int*) – Seed for random number generator, used in random bath states sampling.

  Default is **None**.

- **masked** (*bool*) – True if mask numerically unstable points (with coherence > 1) in the averaging over bath states.

  Note: It is up to user to check whether the possible instability is due to numerical error or unphysical assumptions of the calculations.

  Default is **True** for coherence calculations, **False** for noise calculations.

- **parallel_states** (*bool*) – True if to use MPI to parallelize the calculations of density matrix equally over present mpi processes for random bath state sampling calculations.

  Compared to `parallel` keyword, when this argument is True each process is given a fraction of random bath states. This makes the implementation faster. Works best when the number of bath states is divisible by the number of processes, `nbstates % size == 0`.

  Default is **False**.

- **second_order** (*bool*) – True if add second order perturbation theory correction to the cluster Hamiltonian in conventional CCE. Relevant only for conventional CCE calculations.

  If set to True sets the qubit states as eigenstates of central spin Hamiltonian from the following procedure. If qubit states are provided as vectors in S_z basis, for each qubit state compute the fidelity of the qubit state and all eigenstates of the central spin and chose the one with fidelity higher than `level_confidence`. If such state is not found, raises an error.

  > **Warning:** Second order corrections are not implemented as mean field.
  >
  > I.e., setting `second_order=True` and `nbstates != 0` leads to the calculation, when mean field effect is accounted only from dipolar interactions within the bath.

  Default is **False**.

- **level_confidence** (*float*) – Maximum fidelity of the qubit state to be considered eigenstate of the central spin Hamiltonian.

  Default is 0.95.

- **direct** (*bool*) – True if use direct approach (requires way more memory but might be more numerically stable). False if use memory efficient approach.

  Default is **False**.

- **parallel** (*bool*) – True if parallelize calculation of cluster contributions over different mpi processes.

  Default is **False**.

- **Returns** – ndarray: Computed property.

6.4 Pulse sequences

Documentation of the `Pulse` and `Sequence` classes, used in definition of the complicated pulse sequences.

class BasePulse(*x=None*, *y=None*, *z=None*)

Base class for Pulse.

Parameters

- **x** (*float*) – Rotation angle about x-axis in radians.
- **y** (*float*) – Rotation angle about y-axis in radians.
- **z** (*float*) – Rotation angle about z-axis in radians.

set_angle(*axis*, *angle*)

Set rotation angle `angle` about axis `axis`.

Parameters

- **axis** (*str*) – Axis of the rotation.
- **angle** (*float*) – Rotation angle in radians.

Returns:

check_flip()

Check if the rotation is about single cartesian axis by an angle π.

property naxes

Number of axes the rotation is defined for.

Type
int

property flip

True if the angle == pi.

Type
bool

property x

Angle of rotation of the spin about x axis in rad.

Type
float

property y

Angle of rotation of the spin about y axis in rad.

Type
float

property z

Angle of rotation of the spin about z axis in rad.

Type
float

generate_rotation(*spinvec*, *spin_half=False*)

Generate rotation matrix given spin vector.

Parameters

- **spinvec** (*ndarray with shape (3, n, n)*) – Spin vector.
- **spin_half** (*bool*) – True if spin vector is for a spin-1/2. Default is False.

Returns
Rotation operator.

Return type
ndarray with shape (n, n)

class Pulse(*axis=None*, *angle=None*, *delay=None*, *which=None*, *bath_names=None*, *bath_axes=None*, *bath_angles=None*, ***kwargs*)

Class containing properties of each control pulse, applied to the system.

The properties of the pulse, applied on the central spin(s) can be accessed as attributes, while bath spin pulses can be acessed as elements of the `Pulse` instance.

Parameters

- **axis** (*str*) – Axis of rotation of the central spin. Can be 'x', 'y', or 'z'. Default is None.

- **angle** (*float or str*) – Angle of rotation of central spin. Can be provided in rad, or as a string, containing fraction of pi: `'pi'`, `'pi/2'`, `'2*pi'` etc. Default is None.
- **delay** (*float or ndarray*) – Delay before the pulse or array of delays with the same shape as time points. Default is None.
- **which** (*array-like*) – Indexes of the central spins to be rotated by the pulse. Default is all. Separated indexes are supported only if qubit states are provided separately for all center spins.
- **bath_names** (*str or array-like of str*) – Name or array of names of bath spin types, impacted by the bath pulse. Default is None.
- **bath_axes** (*str or array-like of str*) – Axis of rotation or array of axes of the bath spins. Default is None. If `bath_names` is provided, but `bath_axes` and `bath_angles` are not, assumes the same axis and angle as the one of the central spin
- **bath_angles** (*float or str or array-like*) – Angle of rotation or array of axes of rotations of the bath spins.
- **x** (*float*) – Rotation angle of the central spin about x-axis in radians.
- **y** (*float*) – Rotation angle of the central spin about y-axis in radians.
- **z** (*float*) – Rotation angle of the central spin about z-axis in radians.

Examples

```
>>> Pulse('x', 'pi')
Pulse((x: 3.14, y: 0.00, z: 0.00))
>>> Pulse('x', 'pi', bath_names=['13C', '14C'])
Pulse((x: 3.14, y: 0.00, z: 0.00), {13C: (x: 3.14, y: 0.00, z: 0.00), 14C: (x: 3.14,
↪ y: 0.00, z: 0.00)})
>>> import numpy as np
>>> p = Pulse('x', 'pi', delay=np.linspace(0, 1, 5), bath_names=['13C', '14C'],
>>>           bath_axes='x', bath_angles='pi/2')
>>> print(p)
Pulse((x: 3.14, y: 0.00, z: 0.00), {13C: (x: 1.57, y: 0.00, z: 0.00), 14C: (x: 1.57,
↪ y: 0.00, z: 0.00)},
t = [0.   0.25 0.5  0.75 1.  ])
>>> print(p['13C'])
(x: 1.57, y: 0.00, z: 0.00)
```

which

Indexes of the central spins to be rotated by the pulse.

Type
iterable

bath_names

Array of names of bath spin types, impacted by the bath pulse.

Type
ndarray

bath_axes

Array of axes of rotation of the bath spins.

Type
ndarray

`bath_angles`

Array of angles of rotation of the bath spins.

Type
ndarray

`rotation`

Matrix representation of the pulse for the given cluster. Generated by `Run` object.

Type
ndarray

`property delay`

Delay or array of delays before the pulse.

Type
ndarray or float

`class Sequence(t=None)`

List-like object, which contains the sequence of the pulses.

Each element is a `Pulse` instance, which can be generated from either the tuple with positional arguments or from the dictionary, or set manually.

If delay is not provided in **all** pulses in the sequence, assume equispaced pulse sequence:

t - pulse - 2t - pulse - 2t - … - pulse - t

If only **some** delays are provided, assumes 0 delay in the pulses without delay provided.

Examples

```
>>> import numpy as np
>>> Sequence([('x', np.pi, 0),
>>>           {'axis': 'y', 'angle': 'pi', 'delay': np.linspace(0, 1, 3), 'bath_
↪names': '13C'},
>>>           Pulse('x', 'pi', 1)])
[Pulse((x, 3.14), t = 0), Pulse((y, 3.14), {13C: (y, 3.14)}, t = [0.  0.5 1. ]),␣
↪Pulse((x, 3.14), t = 1)]
```

`append(item)`

S.append(value) – append value to the end of the sequence

CHAPTER

SEVEN

HAMILTONIAN PARAMETERS INPUT

The default total Hamiltonian of the system is set as:

$$\hat{H} = \hat{H}_S + \hat{H}_{SB} + \hat{H}_B$$

with

$$\hat{H}_S = \sum_i (\mathbf{S}_i \mathbf{D}_i \mathbf{S}_i + \mathbf{B}\gamma_{S_i}\mathbf{S}_i + \sum_{i<j} \mathbf{S}_i \mathbf{K}_{ij} \mathbf{S}_j)$$

$$\hat{H}_{SB} = \sum_{i,k} \mathbf{S}_i \mathbf{A}_{ik} \mathbf{I}_k$$

$$\hat{H}_B = \sum_k \mathbf{I}_k \mathbf{P}_k \mathbf{I}_k + \mathbf{B}\gamma_k \mathbf{I}_k + \sum_{k<l} \mathbf{I}_k \mathbf{J}_{kl} \mathbf{I}_l$$

Where $\hat{H}_S$ is the Hamiltonian of the free central spin, $\hat{H}_{SB}$ denotes interactions between central spin and bath spin, nd $\hat{H}_B$ are intrinsic bath spin interactions:

- $\mathbf{D}$ ($\mathbf{P}$) is the self interaction tensor of the central spin (bath spin). For the electron spin, corresponds to the Zero field splitting (ZFS) tensor. For nuclear spins corresponds to the quadrupole interactions tensor.
- γ_i‘ is the magnetic field interaction tensor of the i-spin describing the interaction of the spin and the external magnetic field.
- $\mathbf{A}$ is the interaction tensor between central and bath spins. In the case of nuclear spin bath, corresponds to the hyperfine couplings.
- $\mathbf{J}$ ($\mathbf{K}$) is the interaction tensor between bath (center) spins.

Each of this terms and additional terms of the Hamiltonian can be defined within **PyCCE** framework as following.

In general, central spin properties are stored in the `CenterArray` instance, bath properties are stored in the `BathArray` instance.

7.1 Central Spin Hamiltonian

The central spin Hamiltonian is provided as attributes of the `CenterArray` object:

- $\mathbf{D}$ is set with `CenterArray.set_zfs` method or during the initialization of the `Simulator` object either from observables *D* and *E* of the zero field splitting **OR** directly as tensor for the interaction $\mathbf{SDS}$ in kHz. By default is zero.

  Examples:

```
>>> c = CenterArray(spin=1)
>>> print(c[0].zfs)
[[0. 0. 0.]
 [0. 0. 0.]
 [0. 0. 0.]]
>>> c[0].set_zfs(D=1e6)
>>> print(c[0].zfs)
[[-333333.33333       0.            0.      ]
 [      0.       -333333.33333       0.      ]
 [      0.            0.       666666.66667]]
```

- γ_S, the tensor describing the interaction of the spin and the external magnetic field in units of gyromagnetic ratio $\mathrm{rad}\cdot\mathrm{kHz}\cdot\mathrm{G}^{-1}$. By default is equal to the gyromagnetic ratio of the free electron spin, $-17609\,\mathrm{rad}\cdot\mathrm{ms}^{-1}\cdot\mathrm{G}^{-1}$.

  For the electron spin, it is proportional to g-tensor $\mathbf{g}$ as:

  $$\gamma_S = \mathbf{g}\frac{\mu_B}{\hbar},$$

  where μ_B is Bohr magneton.

  For the nuclear central spin, it is proportional to the chemical shift tensor σ and gyromagnetic ratio γ as:

  $$\gamma_S = \gamma(1-\sigma)$$

  Examples:

```
>>> c = CenterArray(spin=1)
>>> print(c[0].gyro)
-17608.59705
```

Note: While all other coupling parameters are given in the units of frequency, the gyromagnetic ratio (and therefore tensors coupling magnetic field with the spin) are conventionally given in the units of **angular** frequency and differ by 2π.

- $\mathbf{K}$ is set with `CenterArray.add_interaction` method or by calling `CenterArray.point_dipole` method, assuming the interactions as the ones between magnetic point dipoles.

The magnetic field is set with with `Simulator.set_magnetic_field` method or during the initialization of the `Simulator` object in Gauss (G).

User-defined terms of the single-particle central spin Hamiltonian can be added by adding entries to the `Center.h` attribute (Separate for each `Center` object in `CenterArray`).

For example, to add Stevens operator $B_k^q\hat{O}_k^q = 3\hat{S}_z - s(s+1)\hat{I}$ with $q=0$, $k=2$, and $B_k^q = 1\mathrm{GHz}$ to the central spin Hamiltonian, one needs to add:

```
>>> c = CenterArray(spin=1)
>>> k, q = 2, 0
>>> c.h[k, q] = 1e6 # in KHz
```

For details see `Center` documentation.

7.2 Spin-Bath Hamiltonian

The interactions between central spin and bath spins and are provided in the `.A` attribute of the `BathArray` object in kHz.

Interaction tensors can be either:

- Directly provided by setting the values of `bath.A` in kHz for each bath spin.
- Approximated from magnetic point dipole–dipole interactions by calling `BathArray.from_point_dipole` method. Then the tensors are computed as:

$$\mathbf{A}_j = -\gamma_S \gamma_j \frac{\hbar^2}{4\pi\mu_0} \left[\frac{3\vec{r_j} \otimes \vec{r_j} - |r_{ij}|^2 I}{|r_j|^5} \right]$$

  Where γ_j is gyromagnetic ratio of j spin, $\vec{r_j}$ is position of the bath spin, and I is 3x3 identity matrix. The default option when reading the bath by `Simulator` object.

- Approximated from the spin density distribution of the central spin by calling `BathArray.from_cube` method.

  Examples:

```
>>> bath = random_bath('13C', size=100, number=5, seed=1)
>>> print(bath)
[('13C', [  1.182,  45.046, -35.584], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]],␣
↪[[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [ 44.865, -18.817,  -7.667], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]],␣
↪[[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [ 32.77 ,  -9.08 ,   4.959], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]],␣
↪[[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [-47.244,  25.351,   3.814], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]],␣
↪[[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [-17.027,  28.843, -19.681], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]],␣
↪[[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])]
>>> bath.A = 1
>>> print(bath)
[('13C', [  1.182,  45.046, -35.584], [[1., 1., 1.], [1., 1., 1.], [1., 1., 1.]],␣
↪[[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [ 44.865, -18.817,  -7.667], [[1., 1., 1.], [1., 1., 1.], [1., 1., 1.]],␣
↪[[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [ 32.77 ,  -9.08 ,   4.959], [[1., 1., 1.], [1., 1., 1.], [1., 1., 1.]],␣
↪[[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [-47.244,  25.351,   3.814], [[1., 1., 1.], [1., 1., 1.], [1., 1., 1.]],␣
↪[[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [-17.027,  28.843, -19.681], [[1., 1., 1.], [1., 1., 1.], [1., 1., 1.]],␣
↪[[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])]
>>> bath.from_point_dipole([0, 0, 0])
>>> print(bath)
[('13C', [  1.182,  45.046, -35.584], [[-0.659,  0.032, -0.025], [ 0.032,  0.559, -
↪0.963], [-0.025, -0.963,  0.1  ]], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [ 44.865, -18.817,  -7.667], [[ 1.558, -1.092, -0.445], [-1.092, -0.588, ␣
↪0.187], [-0.445,  0.187, -0.97 ]], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [ 32.77 ,  -9.08 ,   4.959], [[ 5.32 , -2.327,  1.271], [-2.327, -2.434, -
↪0.352], [ 1.271, -0.352, -2.886]], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
 ('13C', [-47.244,  25.351,   3.814], [[ 1.06 , -1.   , -0.151], [-1.   , -0.268, ␣
↪0.081], [-0.151,  0.081, -0.792]], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])
```

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```
 ('13C', [-17.027,  28.843, -19.681], [[-0.903, -2.081,  1.42 ], [-2.081,  1.393, -
↪2.405], [ 1.42 , -2.405, -0.49 ]], [[0., 0., 0.], [0., 0., 0.], [0., 0., 0.]])]
```

7.3 Bath Hamiltonian

The self interaction tensors of the bath spins is stored in the `.Q` attribute of the `BathArray` object. By default they are set to 0. They can be either:

- Directly provided by setting the values of `bath.Q` in kHz for each bath spin.
- Computed from the electric field gradient (EFG) tensors at each bath spin position, using `BathArray.from_efg` method.

The gyromagnetic ratio γ_j of each bath spin type is stored in the `BathArray.types`.

The couplings between bath spins are assumed to follow point dipole-dipole interactions as:

$$\mathbf{P}_{ij} = -\gamma_i\gamma_j \frac{\hbar^2}{4\pi\mu_0}\left[\frac{3\vec{r_{ij}}\otimes\vec{r_ij} - |r_{ij}|^2 I}{|r_{ij}|^5}\right]$$

Where γ_i is gyromagnetic ratio of *i* tensor, I is 3x3 identity matrix, and $\vec{r_{ij}}$ is distance between two vectors.

However, user can define the interaction tensors for specific bath spin pairs stored in the `BathArray instance. This can be achieved by:

- Calling `BathArray.add_interaction` method of the `BathArray` instance.
- Providing `InteractionsMap` instance as `imap` keyword to the `Simulator.read_bath`.

Examples:

```
>>> import numpy as np
>>> bath = random_bath('13C', size=100, number=5, seed=1)
>>> print(bath.types)
SpinDict(13C: (13C, 0.5, 6.7283))
>>> test_tensor = np.random.random((3, 3))
>>> bath.add_interaction(0, 1, (test_tensor + test_tensor.T) / 2)
>>> print(bath.imap[0, 1])
[[0.786 0.53  0.404]
 [0.53  0.821 0.366]
 [0.404 0.366 0.655]]
>>> print(bath.imap[0, 1])
[[0.786 0.53  0.404]
 [0.53  0.821 0.366]
 [0.404 0.366 0.655]]
```

User-defined terms of the single-particle bath spin Hamiltonian can be added by adding entries to the `BathArray.h` attribute (Separate for each type of bath spin).

For example, to add non-linear term AI_x^4 with $A = 1\text{MHz}$ to the ^{13}C bath spins (which for spin-1/2 is just proportional to identity, but for higher spins can be relevant) to the bath spin Hamiltonian, one needs to add:

```
>>> bath['13C'].h['xxxx'] = 1e3 # in kHz
```

For details see `BathArray` documentation.

CHAPTER

EIGHT

ELECTRONIC STRUCTURE OUTPUT

Each of the interfaces includes the function that should be used to read electronic structure calculations output into `BathArray` instance.

8.1 Quantum Espresso interface

read_qe(*pwfile*, *hyperfine=None*, *efg=None*, *s=1*, *pwtype=None*, *types=None*, *isotopes=None*, *center=None*, *center_type=None*, *rotation_matrix=None*, *rm_style='col'*, *find_isotopes=True*)

Function to read PW/GIPAW output from Quantum Espresso into BathArray.

Changes the names of the atoms to the most abundant isotopes if `find_isotopes` set to True. If that is not the desired outcome, user can define which isotopes to use using keyword isotopes. If `find_isotopes` is False, then keep the original names even when `isotopes` argument is provided.

Parameters

- **pwfile** (*str*) – Name of PW input or output file. If the file doesn't have proper extension, parameter pw_type should indicate the type.
- **hyperfine** (*str*) – name of the GIPAW hyperfine output.
- **efg** (*str*) – Name of the gipaw electric field tensor output.
- **s** (*float*) – Spin of the central spin. Default 1.
- **pwtype** (*str*) – Type of the `pwfile`. if not listed, will be inferred from extension of pwfile.
- **types** (SpinDict *or list of tuples*) – SpinDict containing SpinTypes of isotopes or input to make one.
- **isotopes** (*dict*) – Optional. Dictionary with entries: {"element" : "isotope"}, where "element" is the name of the element in DFT output, "isotope" is the name of the isotope.
- **center** (*ndarray of shape (3,)*) – Position of (0, 0, 0) point in input coordinates.
- **center_type** (*str*) – Type of the coordinates provided in center argument. Possible value include: 'bohr', 'angstrom', 'crystal', 'alat'. Default assumes the same as in PW file.
- **rotation_matrix** (*ndarray of shape (3,3)*) – Rotation matrix to rotate basis. For details see utilities.transform.
- **rm_style** (*str*) – Indicates how rotation matrix should be interpreted. Can take values "col" or "row". Default "col"
- **find_isotopes** (*bool*) – If true, sets isotopes instead of names of the atoms.

Returns
BathArray containing atoms with hyperfine couplings and quadrupole tensors from QE output.

Return type
BathArray

8.2 ORCA interface

read_orca(*fname*, *isotopes=None*, *types=None*, *center=None*, *find_isotopes=True*, *rotation_matrix=None*, *rm_style='col'*)

Function to read ORCA output containing the hyperfines couplings and EFG tensors.

if `find_isotopes` is set to True changes the names of the atoms to the most abundant isotopes. If that is not the desired outcome, user can define which isotopes to use using keyword isotopes.

Parameters

- **fname** (*str*) – file name of the ORCA output.
- **isotopes** (*dict*) – Optional. Dictionary with entries:

```
{"element" : "isotope"}
```

  where "element" is the name of the element in DFT output, "isotope" is the name of the isotope.
- **types** (SpinDict *or list of tuples*) – SpinDict containing SpinTypes of isotopes or input to make one.
- **center** (*ndarray of shape (3,)*) – position of (0, 0, 0) point in the DFT coordinates.
- **rotation_matrix** (*ndarray of shape (3,3)*) – Rotation matrix to rotate basis. For details see utilities.transform.
- **rm_style** (*str*) – Indicates how rotation matrix should be interpreted. Can take values "col" or "row". Default "col"
- **find_isotopes** (*bool*) – If true, sets isotopes instead of names of the atoms.

Returns
Array of bath spins with hyperfine couplings and quadrupole tensors from Orca output.

Return type
BathArray

CHAPTER

NINE

CCE CALCULATORS

Documentation for the calculator objects called by `Simulator` object.

9.1 Base class

class RunObject(*timespace*, *clusters*, *bath*, *magnetic_field*, *center=None*, *pulses=None*, *nbstates=None*, *seed=None*, *masked=True*, *parallel=False*, *direct=False*, *parallel_states=False*, *store_states=False*, *as_delay=False*, ***kwargs*)

Abstract class of the CCE simulation runner.

Implements cluster correlation expansion, interlaced averaging, and sampling over random bath states. Requires definition of the following methods, from which the kernel will be automatically created:

- `.generate_hamiltonian(self)` method which, using the attributes of the `self` object, computes cluster hamiltonian stored in `self.cluster_hamiltonian`.
- `.compute_result(self)` method which, using the attributes of the `self`, computes the resulting quantity for the given cluster.

Alternatively, user can define the kernel manually. Then the following methods have to be overridden:

- `.kernel(self, cluster, *args, **kwargs)` method which takes indexes of the bath spins in the given cluster as a first positional argument. This method is required for usual CCE runs.
- `.interlaced_kernel(self, cluster, supercluster, *args, **kwargs)` method which takes indexes of the bath spins in the given cluster as a first positional argument, indexes of the supercluster as a second positional argument. This method is required for interlaced CCE runs.

Parameters

- **timespace** (*ndarray with shape (t,)*) – Time delay values at which to compute propagators.
- **clusters** (*dict*) – Clusters included in different CCE orders of structure `{int order: ndarray([[i,j],[i,j]])}`.
- **bath** (*BathArray with shape (n,)*) – Array of n bath spins.
- **magnetic_field** (*ndarray*) – Magnetic field of type `magnetic_field = np.array([Bx, By, Bz])`.
- **alpha** (*int or ndarray with shape (2s+1,)*) – 0 state of the qubit in S_z basis or the index of eigenstate to be used as one.
- **beta** (*int or ndarray with shape (2s+1,)*) – 1 state of the qubit in S_z basis or the index of the eigenstate to be used as one.

- **state** (*ndarray with shape (2s+1,)*) – Initial state of the central spin, used in gCCE and noise autocorrelation calculations. Defaults to $\frac{1}{N}(0+1)$ if not set **OR** if alpha and beta are provided as indexes.
- **spin** (*float*) – Value of the central spin.
- **zfs** (*ndarray with shape (3,3)*) – Zero Field Splitting tensor of the central spin.
- **gyro** (*float or ndarray with shape (3, 3)*) – Gyromagnetic ratio of the central spin

  OR

  tensor corresponding to interaction between magnetic field and central spin.
- **as_delay** (*bool*) – True if time points are delay between pulses, False if time points are total time.
- **nbstates** (*int*) – Number of random bath states to sample over in bath state sampling runs.
- **bath_state** (*ndarray*) – Array of bath states in any accepted format.
- **seed** (*int*) – Seed for the random number generator in bath states sampling.
- **masked** (*bool*) – True if mask numerically unstable points (with result > result[0]) in the sampling over bath states False if not. Default True.
- **projected_bath_state** (*ndarray with shape (n,)*) – Array with z-projections of the bath spins states. Overridden in runs with random bath state sampling.
- **parallel** (*bool*) – True if parallelize calculation of cluster contributions over different mpi processes. Default False.
- **direct** (*bool*) – True if use direct approach in run (requires way more memory but might be more numerically stable). False if use memory efficient approach. Default False.
- **parallel_states** (*bool*) – True if use MPI to parallelize the calculations of density matrix for each random bath state.
- ****kwargs** – Additional keyword arguments to be set as the attributes of the given object.

result_operator(*b*, */*)

Operator which will combine the result of expansion,.

Default: `operator.imul`.

contribution_operator(*b*, */*)

Operator which will combine multiple contributions of the same cluster in the optimized approach.

Default: `operator.ipow`.

removal_operator(*b*, */*)

Operator which will remove subcluster contribution from the given cluster contribution. First argument cluster contribution, second - subcluster contribution.

Defalut: `operator.itruediv`.

addition_operator(*axis=None*, *dtype=None*, *out=None*, *keepdims=<no value>*, *initial=<no value>*, *where=<no value>*)

Group operation which will combine contributions from the different clusters into one contribution in the direct approach.

Default: `numpy.prod`.

nbstates

Number of random bath states to sample over in bath state sampling runs.

Type
int

timespace

Time points at which result will be computed.

Type
ndarray with shape (t,)

clusters

Clusters included in different CCE orders of structure `{int order: ndarray([[i,j],[i,j]])}`.

Type
dict

bath

Array of *n* bath spins.

Type
BathArray with shape (n,)

center

Properties of the central spin.

Type
CenterArray

magnetic_field

Magnetic field of type `magnetic_field = np.array([Bx, By, Bz])`, or a function that takes position as an argument.

Type
ndarray or callable

as_delay

True if time points are delay between pulses, False if time points are total time.

Type
bool

parallel

True if parallelize calculation of cluster contributions over different mpi processes. Default False.

Type
bool

parallel_states

True if use MPI to parallelize the calculations of density matrix for each random bath state.

Type
bool

direct

True if use direct approach in run (requires way more memory but might be more numerically stable). False if use memory efficient approach. Default False.

Type
bool

seed

Seed for the random number generator in bath states sampling.

Type
int

masked

True if mask numerically unstable points (with result > result[0]) in the sampling over bath states False if not. Default True.

Type
bool

store_states

True if store the intermediate state of the cluster. Default False.

Type
bool

cluster_evolved_states

State of the cluster after the evolution

Type
ndarray or bool

hamiltonian

Full cluster Hamiltonian.

Type
ndarray

cluster

Array of the bath spins inside the given cluster.

Type
BathArray

has_states

Whether there are states provided in the bath during the run.

Type
bool

initial_states_mask

Bool array of the states, initially present in the bath.

Type
ndarray

pulses

Sequence object, containing series of pulses, applied to the system.

Type
Sequence

projected_states

Array of S_z projections of the bath spins after each control pulse, involving bath spins.

Type
ndarray

base_hamiltonian

Hamiltonian of the given cluster without mean field additions. In conventional CCE, also excludes additions from central spins.

Type
Hamiltonian

result

Result of the calculation.

Type
ndarray

delays

List with delays before each pulse or None if equispaced. Generated by `.generate_pulses` method.

Type
list or None

rotations

List with matrix representations of the rotation from each pulse. Generated by `.generate_pulses` method.

Type
list

preprocess()

Method which will be called before cluster-expanded run.

postprocess()

Method which will be called after cluster-expanded run.

kernel(*cluster*, **args*, ***kwargs*)

Central kernel that will be called in the cluster-expanded calculations.

Parameters

- **cluster** (*ndarray*) – Indexes of the bath spins in the given cluster.
- ***args** – Positional arguments of the kernel.
- ****kwargs** – Keyword arguments of the kernel.

Returns
Results of the calculations.

Return type
ndarray

run_with_total_bath(**args*, ***kwargs*)

Numerical simulation using the full bath. Emulates kernel with preprocess and postprocess added.

Parameters

- ***args** – Positional arguments of the kernel.
- ****kwargs** – Keyword arguments of the kernel.

Returns
Results of the calculations.

Return type
ndarray

run(**args*, ***kwargs*)

Method that runs cluster-expanded single calculation.

Parameters

- ***args** – Positional arguments of the kernel.
- ****kwargs** – Keyword arguments of the kernel.

Returns
Results of the calculations.

Return type
ndarray

sampling_run(**args*, ***kwargs*)

Method that runs bath sampling calculations.

Parameters

- ***args** – Positional arguments of the kernel.
- ****kwargs** – Keyword arguments of the kernel.

Returns
Results of the calculations.

Return type
ndarray

interlaced_kernel(*cluster*, *supercluster*, **args*, ***kwargs*)

Central kernel that will be called in the cluster-expanded calculations with interlaced averaging of bath spin states.

Parameters

- **cluster** (*ndarray*) – Indexes of the bath spins in the given cluster.
- **supercluster** (*ndarray*) – Indexes of the bath spins in the supercluster of the given cluster. Supercluster is the union of all clusters in `.clusters` attribute, for which given cluster is a subset.
- ***args** – Positional arguments of the kernel.
- ****kwargs** – Keyword arguments of the kernel.

Returns
Results of the calculations.

Return type
ndarray

interlaced_run(**args*, ***kwargs*)

Method that runs cluster-expanded single calculation with interlaced averaging of bath spin states.

Parameters

- ***args** – Positional arguments of the interlaced kernel.
- ****kwargs** – Keyword arguments of the interlaced kernel.

Returns
Results of the calculations.

Return type
ndarray

sampling_interlaced_run(**args*, ***kwargs*)

Method that runs bath sampling calculations with interlaced averaging of bath spin states.

Parameters

- ***args** – Positional arguments of the interlaced kernel.
- ****kwargs** – Keyword arguments of the interlaced kernel.

Returns
Results of the calculations.

Return type
ndarray

classmethod from_simulator(*sim*, ***kwargs*)

Class method to generate `RunObject` from the properties of `Simulator` object.

Parameters

- **sim** (`Simulator`) – Object, whose properties will be used to initialize `RunObject` instance.
- ****kwargs** – Additional keyword arguments that will replace ones, recovered from the `Simulator` object.

Returns
New instance of `RunObject` class.

Return type
RunObject

generate_supercluser_states(*supercluster*)

Helper function to generate all possible pure states of the given supercluster.

Parameters
supercluster (*ndarray with shape (n,)*) – Indexes of the bath spins in the supercluster.

Yields
ndarray with shape (n,) – Pure state of the given supercluster.

generate_pulses()

Generate list of matrix representations of the rotations, induced by the sequence of the pulses.

Returns

tuple containing:

- **list** or **None**: List with delays before each pulse or None if equispaced.
- **list**: List with matrix representations of the rotation from each pulse.

Return type
tuple

get_hamiltonian_variable_bath_state(*index=0*)

Generate Hamiltonian in case of the complicated pulse sequence.

Parameters
index (*int*) – Index of the flips of spin states.

Returns
Hamiltonian with mean field additions from the given set of projected states.

Return type
ndarray with shape (n, n)

`from_sigma`(*sigma*, *i*, *dims*)

Generate spin vector from dictionary with spin matrices.

Parameters

- **sigma** (*dict*) – Dictionary, which contains spin matrices of form `{'x': Sx, 'y': Sy, 'z': Sz}`.
- **i** (*int*) – Index of the spin in the order of `dims`.
- **dims** (*ndarray with shape (N,)*) – Dimensions of the spins in the given cluster.

Returns
Spin vector in a full Hilbert space.

Return type
ndarray with shape (3, n, n)

`generate_rotated_projected_states`(*bath*, *pulses*)

Generate projected states after each control pulse, involving bath spins.

Parameters

- **bath** (*BathArray with shape (n,)*) – Array of bath spins.
- **pulses** (Sequence) – Sequence of pulses.

Returns
Array of S_z projections of bath spin states after each pulse, involving bath spins. Each i-th column is projections before the i-th pulse involving bath spins.

Return type
ndarray with shape (n, x)

`pulse_bath_rotation`(*pulse*, *vectors*)

Generate rotation of the bath spins from the given pulse.

Parameters

- **pulse** (Pulse) – Control pulse.
- **vectors** (*ndarray with shape (n, 3, N, N)*) – Array of spin vectors.

Returns
Matrix representation of the spin rotation.

Return type
ndarray with shape (x, x)

`simple_propagator`(*timespace*, *hamiltonian*)

Generate a simple propagator $U = \exp[-\frac{i}{\hbar}\hat{H}]$ from the Hamiltonian.

Parameters

- **timespace** (*ndarray with shape (n,)*) – Time points at which to evaluate the propagator.
- **hamiltonian** (*ndarray with shape (N, N)*) – Hamiltonian of the system.

Returns
Propagators, evaluated at each timepoint.

Return type
ndarray with shape (n, N, N)

from_central_state(*dimensions*, *central_state*)

Generate density matrix of the system if all spins apart from central spin are in completely mixed state.

Parameters

- **dimensions** (*ndarray with shape (n,)*) – Array of the dimensions of the spins in the cluster.
- **central_state** (*ndarray with shape (x,)*) – Density matrix of central spins.

Returns
Density matrix for the whole cluster.

Return type
ndarray with shape (N, N)

from_none(*dimensions*)

Generate density matrix of the systems if all spins are in completely mixed state. :param dimensions: Array of the dimensions of the spins in the cluster. :type dimensions: ndarray with shape (n,)

Returns
Density matrix for the whole cluster.

Return type
ndarray with shape (N, N)

from_states(*states*)

Generate density matrix of the systems if all spins are in pure states. :param states: Array of the pure spin states. :type states: array-like

Returns
Spin vector for the whole cluster.

Return type
ndarray with shape (N, N)

combine_cluster_central(*cluster_state*, *central_state*)

Combine bath spin states and the state of central spin. :param cluster_state: State vector or density matrix of the bath spins. :type cluster_state: ndarray with shape (n,) or (n, n) :param central_state: State vector or density matrix of the central spins. :type central_state: ndarray with shape (m,) or (m, m)

Returns
State vector or density matrix of the full system.

Return type
ndarray with shape (mn,) or (mn, mn)

rand_state(*d*)

Generate random state of the spin.

Parameters
d (*int*) – Dimensions of the spin.

Returns
Density matrix of the random state.

Return type
ndarray with shape (d, d)

generate_initial_state(*dimensions*, *states=None*, *central_state=None*)

Generate initial state of the cluster.

Parameters

- **dimensions** (*ndarray with shape (n,)*) – Dimensions of all spins in the cluster.
- **states** (*BathState, optional*) – States of the bath spins. If None, assumes completely random state.
- **central_state** (*ndarray*) – State of the central spin. If None, assumes that no central spin is present in the Hilbert space of the cluster.

Returns

State vector or density matrix of the cluster.

Return type

ndarray with shape (N,) or (N, N)

9.2 Conventional CCE

simple_propagators(*delays*, *hamiltonian_alpha*, *hamiltonian_beta*)

Generate two simple propagators $U = \exp[-\frac{i}{\hbar}\hat{H}]$ from the Hamiltonians, conditioned on two qubit levels.

Parameters

- **delays** (*ndarray with shape (n,)*) – Time points at which to evaluate the propagator.
- **hamiltonian_alpha** (*ndarray with shape (N, N)*) – Hamiltonian of the bath spins with qubit in alpha state.
- **hamiltonian_beta** (*ndarray with shape (N, N)*) – Hamiltonian of the bath spins with qubit in beta state.

Returns

- **ndarray with shape (n, N, N)**: Matrix representation of the propagator conditioned on the alpha qubit state for each time point.
- **ndarray with shape (n, N, N)**: Matrix representation of the propagator conditioned on the beta qubit state for each time point.

Return type

tuple

propagate_propagators(*v0*, *v1*, *number*)

From two simple propagators and number of pulses in CPMG sequence generate two full propagators. :param v0: Propagator conditioned on the alpha qubit state for each time point. :type v0: ndarray with shape (n, N, N) :param v1: Propagator conditioned on the beta qubit state for each time point. :type v1: ndarray with shape (n, N, N) :param number: Number of pulses. :type number: int

Returns

- **ndarray with shape (n, N, N)**: Matrix representation of the propagator conditioned on the alpha qubit state for each time point.
- **ndarray with shape (n, N, N)**: Matrix representation of the propagator conditioned on the beta qubit state for each time point.

Return type

tuple

class CCE(**args*, *second_order=False*, *level_confidence=0.95*, ***kwargs*)

Class for running conventional CCE simulations.

Note: Subclass of the `RunObject` abstract class.

Parameters

- ***args** – Positional arguments of the `RunObject`.
- **pulses** (*int or* `Sequence`) – number of pulses in CPMG sequence or instance of Sequence object. For now, only CPMG sequences are supported in conventional CCE simulations.
- **second_order** (*bool*) – True if add second order perturbation theory correction to the cluster Hamiltonian. If set to True sets the qubit states as eigenstates of central spin Hamiltonian from the following procedure. If qubit states are provided as vectors in S_z basis, for each qubit state compute the fidelity of the qubit state and all eigenstates of the central spin and chose the one with fidelity higher than `level_confidence`. If such state is not found, raises an error.
- **level_confidence** (*float*) – Maximum fidelity of the qubit state to be considered eigenstate of the central spin Hamiltonian. Default 0.95.
- ****kwargs** – Keyword arguments of the `RunObject`.

initial_pulses

Input pulses

Type
int or *Sequence*

pulses

If input Sequence contains only pi pulses at even delay, stores number of pulses. Otherwise stores full `Sequence`.

Type
int or *Sequence*

second_order

True if add second order perturbation theory correction to the cluster hamiltonian.

Type
bool

level_confidence

Maximum fidelity of the qubit state to be considered eigenstate of the central spin hamiltonian.

Type
float

energy_alpha

Eigen energy of the alpha state in the central spin Hamiltonian.

Type
float

`energy_beta`

Eigen energy of the beta state in the central spin Hamiltonian.

Type
float

`energies`

All eigen energies of the central spin Hamiltonian.

Type
ndarray with shape (2s+1,)

`projections_alpha_all`

Array of vectors with spin operator matrix elements of type $[0\hat{S}_x i, 0\hat{S}_y i, 0\hat{S}_z i]$, where 0 is the alpha qubit state, i are all eigenstates of the central spin hamiltonian.

Type
ndarray with shape (2s+1, 3)

`projections_beta_all`

Array of vectors with spin operator matrix elements of type $[1\hat{S}_x i, 1\hat{S}_y i, 1\hat{S}_z i]$, where 1 is the beta qubit state, i are all eigenstates of the central spin hamiltonian.

Type
ndarray with shape (2s+1, 3)

`projections_alpha`

Vector with spin operator matrix elements of type $[0\hat{S}_x 0, 0\hat{S}_y 0, 0\hat{S}_z 0]$, where 0 is the alpha qubit state

Type
ndarray with shape (3,)

`projections_beta`

Vectors with spin operator matrix elements of type $[1\hat{S}_x 1, 1\hat{S}_y 1, 1\hat{S}_z 1]$, where 1 is the beta qubit state.

Type
ndarray with shape (3,)

`use_pulses`

True if use full `Sequence`. False if use only number of pulses.

Type
bool

`preprocess()`

Method which will be called before cluster-expanded run.

`postprocess()`

Method which will be called after cluster-expanded run.

`generate_hamiltonian()`

Using the attributes of the `self` object, compute the two projected cluster hamiltonians.

Returns

Tuple containing:

- **Hamiltonian**: Cluster hamiltonian when qubit in the alpha state.
- **Hamiltonian**: Cluster hamiltonian when qubit in the alpha state.

Return type
tuple

`compute_result()`

Using the attributes of the `self` object, compute the coherence function as overlap in the bath evolution.

Returns
Computed coherence.

Return type
ndarray

`propagators()`

Generate two propagators, conditioned on the qubit state.

Returns

tuple containing:

- **ndarray with shape (t, n, n)**: Matrix representation of the propagator conditioned on the alpha qubit state for each time point.
- **ndarray with shape (t, n, n)**: Matrix representation of the propagator conditioned on the beta qubit state for each time point.

Return type
tuple

9.3 Generalized CCE

`rotation_propagator(`u, *rotations*`)`

Generate the propagator from the simple propagator and set of $2au$ equispaced rotation operators.

Note: While the spacing between rotation operators is assumed to be $2au$, the spacing before and after the first and the last rotation respectively is assumed to be :math:` au`.

Parameters

- **u** (*ndarray with shape (n, N, N)*) – Simple propagator.
- **rotations** (*ndarray with shape (x, N, N)*) – Array of rotation operators.

Returns
Full propagator.

Return type
ndarray with shape (n, N, N)

`class gCCE(`**args*, *i=None*, *j=None*, *fulldm=False*, *normalized=True*, ***kwargs*`)`

Class for running generalized CCE simulations.

Note: Subclass of the `RunObject` abstract class.

Parameters

- ***args** – Positional arguments of the `RunObject`.
- **pulses** (`Sequence`) – Sequence object, containing series of pulses, applied to the system.
- **fulldm** (*bool*) – True if return full density matrix. Default False.
- ****kwargs** – Keyword arguments of the `RunObject`.

dm0

Initial density matrix of the central spin.

Type
ndarray with shape (2s+1, 2s+1)

normalization

Coherence at time 0.

Type
float

zero_cluster

Coherence computed for the isolated central spin.

Type
ndarray with shape (n,)

fulldm

True if return full density matrix.

Type
bool

preprocess()

Method which will be called before cluster-expanded run.

process_dm(*density_matrix*)

Obtain the result from the density matrices.

Parameters
density_matrix (*ndarray with shape (n, N, N)*) – Array of the density matrices.

Returns
Depending on the parameters, returns the off diagonal element of the density matrix or full matrix.

Return type
ndarray

postprocess()

Method which will be called after cluster-expanded run.

generate_hamiltonian()

Using the attributes of the `self` object, compute the cluster hamiltonian including the central spin.

Returns
Cluster hamiltonian.

Return type
Hamiltonian

`compute_result()`

Using the attributes of the `self` object, compute the coherence function of the central spin.

Returns
Computed coherence.

Return type
ndarray

`propagator()`

Function to compute time propagator U.

Returns
Array of propagators, evaluated at each time point in `self.timespace`.

Return type
ndarray with shape (t, n, n)

9.4 Noise Autocorrelation

`correlation_it_j0(operator_i, operator_j, dm0_expanded, U)`

Function to compute correlation function of the operator i at time t and operator j at time 0

Parameters

- **operator_i** (*ndarray with shape (n, n)*) – Matrix representation of operator i.
- **operator_j** (*ndarray with shape (n, n)*) – Matrix representation of operator j.
- **dm0_expanded** (*ndarray with shape (n, n)*) – Initial density matrix of the cluster.
- **U** (*ndarray with shape (t, n, n)*) – Time evolution propagator, evaluated over t time points.

Returns
Autocorrelation of the z-noise at each time point.

Return type
ndarray with shape (t,)

`compute_correlations(nspin, dm0_expanded, U, central_spin=None)`

Function to compute correlations for the given cluster, given time propagator U.

Parameters

- **nspin** (BathArray) – BathArray of the given cluster of bath spins.
- **dm0_expanded** (*ndarray with shape (n, n)*) – Initial density matrix of the cluster.
- **U** (*ndarray with shape (t, n, n)*) – Time evolution propagator, evaluated over t time points.
- **central_spin** (CenterArray) – Array of central spins.

Returns
correlation of the Overhauser field, induced by the given cluster at each time point.

Return type
ndarray with shape (t,)

class gCCENoise(**args*, ***kwargs*)

Class for running generalized CCE simulations of the noise autocorrelation function.

Note: Subclass of the RunObject abstract class.

Parameters

- ***args** – Positional arguments of the RunObject.
- ****kwargs** – Keyword arguments of the RunObject.

result_operator(*b*, */*)

Overridden operator which will combine the result of expansion: operator.iadd.

contribution_operator(*b*, */*)

Overridden operator which will combine multiple contributions of the same cluster in the optimized approach: operator.imul.

removal_operator(*b*, */*)

Overridden operator which remove subcluster contribution from the given cluster contribution: operator.isub.

addition_operator(*axis=None*, *dtype=None*, *out=None*, *keepdims=<no value>*, *initial=<no value>*, *where=<no value>*)

Overridden group operation which will combine contributions from the different clusters into one contribution in the direct approach: numpy.sum.

preprocess()

Method which will be called before cluster-expanded run.

postprocess()

Method which will be called after cluster-expanded run.

generate_hamiltonian()

Using the attributes of the self object, compute the cluster hamiltonian including the central spin.

Returns
Cluster hamiltonian.

Return type
Hamiltonian

compute_result()

Using the attributes of the self object, compute autocorrelation function of the noise from bath spins in the given cluster.

Returns
Computed autocorrelation function.

Return type
ndarray

class CCENoise(**args*, ***kwargs*)

Class for running conventional CCE simulations of the noise autocorrelation function.

Note: Subclass of the RunObject abstract class.

Warning: In general, for calculations of the autocorrelation function, better results are achieved with generalized CCE, which accounts for the evolution of the entangled state of the central spin.

Second order couplings between nuclear spins are not implemented.

Parameters

- ***args** – Positional arguments of the `RunObject`.
- ****kwargs** – Keyword arguments of the `RunObject`.

`result_operator`(*b*, */*)

Overridden operator which will combine the result of expansion: `operator.iadd`.

`contribution_operator`(*b*, */*)

Overridden operator which will combine multiple contributions of the same cluster in the optimized approach: `operator.imul`.

`removal_operator`(*b*, */*)

Overridden operator which remove subcluster contribution from the given cluster contribution: `operator.isub`.

`addition_operator`(*axis=None*, *dtype=None*, *out=None*, *keepdims=<no value>*, *initial=<no value>*, *where=<no value>*)

Overridden group operation which will combine contributions from the different clusters into one contribution in the direct approach: `numpy.sum`.

`preprocess`()

Method which will be called before cluster-expanded run.

`postprocess`()

Method which will be called after cluster-expanded run.

`generate_hamiltonian`()

Using the attributes of the `self` object, compute the projected cluster hamiltonian, averaged for two qubit states.

Returns
Cluster hamiltonian.

Return type
Hamiltonian

`compute_result`()

Using the attributes of the `self` object, compute autocorrelation function of the noise from bath spins in the given cluster.

Returns
Computed autocorrelation function.

Return type
ndarray

9.5 Cluster-correlation Expansion Decorators

The way we find cluster in the code.

generate_clusters(*bath*, *r_dipole*, *order*, *r_inner=0*, *ignore=None*, *strong=False*, *nclusters=None*)

Generate clusters for the bath spins.

Parameters

- **bath** (BathArray) – Array of bath spins.
- **r_dipole** (*float*) – Maximum connectivity distance.
- **order** (*int*) – Maximum size of the clusters to find.
- **r_inner** (*float*) – Minimum connectivity distance.
- **ignore** (*list or str, optional*) – If not None, includes the names of bath spins which are ignored in the cluster generation.
- **strong** (*bool*) – Whether to find only completely interconnected clusters (default False).
- **nclusters** (*dict*) – Dictionary which contain maximum number of clusters of the given size. Has the form `n_clusters = {order: number}`, where `order` is the size of the cluster, `number` is the maximum number of clusters with this size.

  If provided, sorts the clusters by the strength of cluster interaction, equal to the lowest pairwise interaction in the cluster. Then the strongest `number` of clusters is taken.

Returns

Dictionary with keys corresponding to size of the cluster, and value corresponds to ndarray of shape (matrix, N). Here matrix is the number of clusters of given size, N is the size of the cluster. Each row contains indexes of the bath spins included in the given cluster.

Return type

dict

make_graph(*bath*, *r_dipole*, *r_inner=0*, *ignore=None*, *max_size=5000*)

Make a connectivity matrix for bath spins.

Parameters

- **bath** (BathArray) – Array of bath spins.
- **r_dipole** (*float*) – Maximum connectivity distance.
- **r_inner** (*float*) – Minimum connectivity distance.
- **ignore** (*list or str, optional*) – If not None, includes the names of bath spins which are ignored in the cluster generation.
- **max_size** (*int*) – Maximum size of the bath before less optimal (but less memory intensive) approach is used.

Returns

Connectivity matrix.

Return type

crs_matrix

connected_components(*csgraph*, *directed=False*, *connection='weak'*, *return_labels=True*)

Find connected components using `scipy.sparse.csgraph`. See documentation of `scipy.sparse.csgraph.connected_components`

find_subclusters(*maximum_order*, *graph*, *labels*, *n_components*, *strong=False*)

Find subclusters from connectivity matrix.

Parameters

- **maximum_order** (*int*) – Maximum size of the clusters to find.
- **graph** (*csr_matrix*) – Connectivity matrix.
- **labels** (*ndarray with shape (n,)*) – Array of labels of the connected components.
- **n_components** (*int*) – The number of connected components n.
- **strong** (*bool*) – Whether to find only completely interconnected clusters (default False).

Returns

Dictionary with keys corresponding to size of the cluster, and value corresponds to ndarray of shape (matrix, N). Here matrix is the number of clusters of given size, N is the size of the cluster. Each row contains indexes of the bath spins included in the given cluster.

Return type

dict

combine_clusters(*cs1*, *cs2*)

Combine two dictionaries with clusters.

Parameters

- **cs1** (*dict*) – First cluster dictionary with keys corresponding to size of the cluster, and value corresponds to ndarray of shape (matrix, N).
- **cs2** (*dict*) – Second cluster dictionary with the same structure.

Returns

Combined dictionary with unique clusters from both dictionaries.

Return type

dict

expand_clusters(*sc*)

Expand dict so each new cluster will include all possible additions of one more bath spin. This increases maximum size of the cluster by one.

Parameters

sc (*dict*) – Initial clusters dictionary.

Returns

Dictionary with expanded clusters.

Return type

dict

find_valid_subclusters(*graph*, *maximum_order*, *nclusters=None*, *bath=None*, *strong=False*, *compute_strength=None*)

Find subclusters from connectivity matrix.

Parameters

- **maximum_order** (*int*) – Maximum size of the clusters to find.
- **graph** (*csr_matrix*) – Connectivity matrix.
- **nclusters** (*dict*) – Dictionary which contain maximum number of clusters of the given size.

- **bath** (BathArray) – Array of bath spins.
- **strong** (*bool*) – Whether to find only completely interconnected clusters (default False).

Returns
Dictionary with keys corresponding to size of the cluster, and value corresponds to ndarray of shape (matrix, N). Here matrix is the number of clusters of given size, N is the size of the cluster. Each row contains indexes of the bath spins included in the given cluster.

Return type
dict

General decorators that are used to expand kernel of the RunObject class or subclasses to the whole bath *via* CCE. This module contains information about the way the cluster expansion is implemented in the package.

cluster_expansion_decorator(*_func=None*, ***, *result_operator=<built-in function imul>*, *contribution_operator=<built-in function ipow>*, *removal_operator=<built-in function itruediv>*, *addition_operator=<function prod>*)

Decorator for creating cluster correlation expansion of the method of RunObject class.

Parameters

- **_func** (*func*) – Function to expand.
- **result_operator** (*func*) – Operator which will combine the result of expansion (default: operator.imul).
- **contribution_operator** (*func*) – Operator which will combine multiple contributions of the same cluster (default: operator.ipow) in the optimized approach.
- **result_operator** – Operator which will combine the result of expansion (default: operator.imul).
- **removal_operator** (*func*) – Operator which will remove subcluster contribution from the given cluster contribution. First argument cluster contribution, second - subcluster contribution (default: operator.itruediv).
- **addition_operator** (*func*) – Group operation which will combine contributions from the different clusters into one contribution (default: np.prod).

Returns
Expanded function.

Return type
func

optimized_approach(*function*, *self*, **arg*, *result_operator=<built-in function imul>*, *contribution_operator=<built-in function ipow>*, ***kwarg*)

Optimized approach to compute cluster correlation expansion.

Parameters

- **function** (*func*) – Function to expand.
- **self** (RunObject) – Object whose method is expanded.
- ***arg** – list of positional arguments of the expanded function.
- **result_operator** (*func*) – Operator which will combine the result of expansion (default: operator.imul).
- **contribution_operator** (*func*) – Operator which will combine multiple contributions of the same cluster (default: operator.ipow).

- ****kwarg** – Dictionary containing all keyword arguments of the expanded function.

Returns
Expanded function.

Return type
func

direct_approach(*function*, *self*, **arg*, *result_operator=<built-in function imul>*, *removal_operator=<built-in function itruediv>*, *addition_operator=<function prod>*, ***kwarg*)

Direct approach to compute cluster correlation expansion.

Parameters

- **function** (*func*) – Function to expand.
- **self** (RunObject) – Object whose method is expanded.
- **result_operator** (*func*) – Operator which will combine the result of expansion (default: operator.imul).
- **removal_operator** (*func*) – Operator which will remove subcluster contribution from the given cluster contribution. First argument cluster contribution, second - subcluster contribution (default: operator.itruediv).
- **addition_operator** (*func*) – Group operation which will combine contributions from the different clusters into one contribution (default: np.prod).
- ****kwarg** – Dictionary containing all keyword arguments of the expanded function.

Returns
Expanded method.

Return type
func

interlaced_decorator(*_func=None*, ***, *result_operator=<built-in function imul>*, *contribution_operator=<built-in function ipow>*)

Decorator for creating interlaced cluster correlation expansion of the method of RunObject class.

Parameters

- **_func** (*func*) – Function to expand.
- **result_operator** (*func*) – Operator which will combine the result of expansion (default: operator.imul).
- **contribution_operator** (*func*) – Operator which will combine multiple contributions of the same cluster (default: operator.ipow) in the optimized approach.

Returns
Expanded method.

Return type
func

Decorators that are used to perform bath state sampling over the kernel of RunObject.

generate_bath_state(*bath*, *nbstates*, *seed=None*, *parallel=False*)

Generator of the random *pure* $\hat{I}_z$ bath eigenstates.

Parameters

- **bath** (BathArray) – Array of bath spins.

- **nbstates** (*int*) – Number of random bath states to generate.
- **seed** (*int*) – Optional. Seed for RNG.
- **parallel** (*bool*) – True if run in parallel mode. Default False.

Yields

List – list of the pure bath spin state vectors.

monte_carlo_method_decorator(*func*)

Decorator to sample over random bath states given function.

CHAPTER

TEN

HAMILTONIAN FUNCTIONS

10.1 Base Class

class Hamiltonian(*dimensions*, *vectors=None*, *data=None*)

Class containing properties of the Hamiltonian.

Essentially wrapper for ndarray with additional attributes of `dimensions` and `spins`.

Usual methods (e.g. `__setitem__` or `__getitem__`) access the `data` attribute.

Note: Algebraic operations with Hamiltonian will return ndarray instance.

Parameters

dimensions (*array-like*) – array of the dimensions for each spin in the Hilbert space of the Hamiltonian.

dimensions

array of the dimensions for each spin in the Hilbert space of the Hamiltonian.

Type
ndarray

spins

array of the spins, spanning the Hilbert space of the Hamiltonian.

Type
ndarray

vectors

list with spin vectors of form `[[Ix, Iy, Iz], [Ix, Iy, Iz], ...]`.

Type
list

data

matrix representation of the Hamiltonian.

Type
ndarray

10.2 Total Hamiltonian

bath_hamiltonian(*bath*, *mfield*)

Compute hamiltonian containing only the bath spins.

Parameters

- **bath** (BathArray) – array of all bath spins in the cluster.
- **mfield** (*ndarray with shape (3,) or func*) – Magnetic field of type `mfield = np.array([Bx, By, Bz])` or callable with signature `mfield(pos)`, where `pos` is ndarray with shape (3,) with the position of the spin.

Returns
Hamiltonian of the given cluster without qubit.

Return type
Hamiltonian

total_hamiltonian(*bath*, *center*, *mfield*)

Compute total Hamiltonian of the given cluster.

Parameters

- **bath** (BathArray) – Array of bath spins.
- **center** (CenterArray) – Array of central spins.
- **mfield** (*ndarray with shape (3,) or func*) – Magnetic field of type `mfield = np.array([Bx, By, Bz])` or callable with signature `mfield(pos)`, where `pos` is ndarray with shape (3,) with the position of the spin.

Returns
hamiltonian of the given cluster, including central spin.

Return type
Hamiltonian

central_hamiltonian(*center*, *magnetic_field*, *hyperfine=None*, *bath_state=None*)

Compute Hamiltonian, containing only central spin.

Parameters

- **center** (CenterArray *or* Center) – Center spin.
- **magnetic_field** (*ndarray with shape (3,) or func*) – Magnetic field of type `magnetic_field = np.array([Bx, By, Bz])` or callable with signature `magnetic_field(pos)`, where `pos` is ndarray with shape (3,) with the position of the spin.
- **hyperfine** (*ndarray with shape (..., n, 3, 3)*) – Array of hyperfine tensors of bath spins.
- **bath_state** (*ndarray with shape (n,)*) – Array of S_z projections of bath spins.

Returns
Central spin Hamiltonian.

Return type
Hamiltonian

custom_hamiltonian(*spins*, *dims=None*, *offset=0*)

Custom addition to the Hamiltonian from the spins in the given array.

Parameters

- **spins** (*BathArray or CenterArray*) – Array of the spins.
- **dims** (*ndarray with shape (n,)*) – Dimensions of all spins in the cluster.
- **offset** (*int*) – Index of the dimensions of the first spin from array in `dims`. Default 0.

Returns
Addition to the Hamiltonian.

Return type
ndarray with shape (N, N)

custom_single(*h*, *index*, *dims*)

Custom addition to the Hamiltonian from the dictionary with the parameters.

Parameters

- **h** (*dict*) – Dictionary with coupling parameters.
- **index** (*int*) – Index of the spin in `dims`.
- **dims** (*ndarray with shape (n,)*) – Dimensions of all spins in the cluster.

Returns
Addition to the Hamiltonian.

Return type
ndarray with shape (N, N)

10.3 Separate Terms

Documentation for the functions used to generate spin Hamiltonian for each cluster.

expanded_single(*ivec*, *gyro*, *mfield*, *self_tensor*, *detuning=0.0*)

Function to compute the single bath spin term.

Parameters

- **ivec** (*ndarray with shape (3, n, n)*) – Spin vector of the bath spin in the full Hilbert space of the cluster.
- **gyro** (*float or ndarray with shape (3, 3)*) –
- **mfield** (*ndarray wtih shape (3,)* – Magnetic field of type `mfield = np.array([Bx, By, Bz])`.
- **self_tensor** (*ndarray with shape (3, 3)*) – tensor of self-interaction of type IPI where I is bath spin.
- **detuning** (*float*) – Additional term of d*Iz allowing to simulate different energy splittings of bath spins.

Returns
Single bath spin term.

Return type
ndarray with shape (n, n)

zeeman(*ivec*, *gyro*, *mfield*)

Function :param ivec: Spin vector of the spin in the full Hilbert space of the cluster. :type ivec: ndarray with shape (3, n, n) :param gyro: Gyromagnetic ratio of the spin. :type gyro: float or ndarray with shape (3, 3) :param mfield: Magnetic field at the position of the spin. :type mfield: ndarray with shape (3,)

Returns
Zeeman interactions.

Return type
ndarray with shape (n, n)

dd_tensor(*coord_1*, *coord_2*, *g1*, *g2*)

Generate dipole-dipole interaction tensor.

Parameters

- **coord_1** (*ndarray with shape (3,)*) – Coordinates of the first spin.
- **coord_2** (*ndarray with shape (3,)*) – Coordinates of the second spin.
- **g1** (*float or ndarray with shape (3, 3)*) – Gyromagnetic ratio of the first spin.
- **g2** (*float or ndarray with shape (3, 3)*) – Gyromagnetic ratio of the second spin.

Returns
Interaction tensor.

Return type
ndarray with shape (3, 3)

dipole_dipole(*coord_1*, *coord_2*, *g1*, *g2*, *ivec_1*, *ivec_2*)

Compute dipole_dipole interactions between two bath spins.

Parameters

- **coord_1** (*ndarray with shape (3,)*) – Coordinates of the first spin.
- **coord_2** (*ndarray with shape (3,)*) – Coordinates of the second spin.
- **g1** (*float*) – Gyromagnetic ratio of the first spin.
- **g2** (*float*) – Gyromagnetic ratio of the second spin.
- **ivec_1** (*ndarray with shape (3, n, n)*) – Spin vector of the first spin in the full Hilbert space of the cluster.
- **ivec_2** (*ndarray with shape (3, n, n)*) – Spin vector of the second spin in the full Hilbert space of the cluster.

Returns
Dipole-dipole interactions.

Return type
ndarray with shape (n, n)

gen_pos_tensor(*coord_1*, *coord_2*)

Generate positional tensor -(3*r @ r.T - r*r), used for hyperfine tensor (without gyro factor).

Parameters

- **coord_1** (*ndarray with shape (3,)*) – Coordinates of the first spin.
- **coord_2** (*ndarray with shape (3,)*) – Coordinates of the second spin.

Returns
Positional tensor.

Return type
ndarray with shape (3, 3)

bath_interactions(*nspin*, *ivectors*)

Compute interactions between bath spins.

Parameters

- **nspin** (BathArray) – Array of the bath spins in the given cluster.
- **ivectors** (*array-like*) – array of expanded spin vectors, each with shape (3, n, n).

Returns
All intrabath interactions of bath spins in the cluster.

Return type
ndarray with shape (n, n)

bath_mediated(*hyperfines*, *ivectors*, *energy_state*, *energies*, *projections*)

Compute all hyperfine-mediated interactions between bath spins.

Parameters

- **hyperfines** (*ndarray with shape (n, 3, 3)*) – Array of hyperfine tensors of the bath spins in the given cluster.
- **ivectors** (*array-like*) – array of expanded spin vectors, each with shape (3, n, n).
- **energy_state** (*float*) – Energy of the qubit state on which the interaction is conditioned.
- **energies** (*ndarray with shape (2s - 1,)*) – Array of energies of all states of the central spin.
- **projections** (*ndarray with shape (2s - 1, 3)*) – Array of vectors of the central spin matrix elements of form:

$$[i\hat{S}_x j, i\hat{S}_y j, i\hat{S}_z j],$$

where i are different states of the central spin.

Returns
Hyperfine-mediated interactions.

Return type
ndarray with shape (n, n)

conditional_hyperfine(*hyperfine_tensor*, *ivec*, *projections*)

Compute conditional hyperfine Hamiltonian.

Parameters

- **hyperfine_tensor** (*ndarray with shape (3, 3)*) – Tensor of hyperfine interactions of the bath spin.
- **ivec** (*ndarray with shape (3, n, n)*) – Spin vector of the bath spin in the full Hilbert space of the cluster.
- **projections** (*ndarray with shape (3,)*) – Array of vectors of the central spin matrix elements of form:

$$[i\hat{S}_x j, i\hat{S}_y j, i\hat{S}_z j],$$

where j are different states of the central spin. If $i = j$, produces the usual conditioned hyperfine interactions and just equal to projections of $\hat{S}_z$ of the central spin state $[\hat{S}_x, \hat{S}_y, \hat{S}_z]$.

If $i \neq j$, gives second order perturbation.

Returns
Conditional hyperfine interaction.

Return type
ndarray with shape (n, n)

hyperfine(*hyperfine_tensor*, *svec*, *ivec*)

Compute hyperfine interactions between central spin and bath spin.

Parameters

- **hyperfine_tensor** (*ndarray with shape (3, 3)*) – Tensor of hyperfine interactions of the bath spin.
- **svec** (*ndarray with shape (3, n, n)*) – Spin vector of the central spin in the full Hilbert space of the cluster.
- **ivec** (*ndarray with shape (3, n, n)*) – Spin vector of the bath spin in the full Hilbert space of the cluster.

Returns
Hyperfine interaction.

Return type
ndarray with shape (n, n)

self_central(*svec*, *mfield*, *tensor*, *gyro=-17608.59705*, *detuning=0*)

Function to compute the central spin term in the Hamiltonian.

Parameters

- **svec** (*ndarray with shape (3, n, n)*) – Spin vector of the central spin in the full Hilbert space of the cluster.
- **mfield** (*ndarray wtih shape (3,)* – Magnetic field of type `mfield = np.array([Bx, By, Bz])`.
- **tensor** (*ndarray with shape (3, 3)*) – Zero Field Splitting tensor of the central spin.
- **gyro** (*float or ndarray with shape (3,3)*) – gyromagnetic ratio of the central spin OR tensor corresponding to interaction between magnetic field and central spin.
- **detuning** (*float*) – Energy detuning from the Zeeman splitting in kHz.

Returns
Central spin term.

Return type
ndarray with shape (n, n)

center_interactions(*center*, *vectors*)

Compute interactions between central spins.

Parameters

- **center** (CenterArray) – Array of central spins
- **vectors** (*ndarray with shape (x, 3, n, n)*) – Array of spin vectors of central spins.

Returns
Central spin Overhauser term.

Return type
ndarray with shape (n, n)

overhauser_central(*svec*, *others_hyperfines*, *others_state*)

Compute Overhauser field term on the central spin from all other spins, not included in the cluster.

Parameters

- **svec** (*ndarray with shape (3, n, n)*) – Spin vector of the central spin in the full Hilbert space of the cluster.
- **others_hyperfines** (*ndarray with shape (m, 3, 3)*) – Array of hyperfine tensors for all bath spins not included in the cluster.
- **others_state** (*ndarray with shape (m,) or (m, 3)*) – Array of I_z projections for each bath spin outside of the given cluster.

Returns
Central spin Overhauser term.

Return type
ndarray with shape (n, n)

overhauser_bath(*ivec*, *position*, *gyro*, *other_gyros*, *others_position*, *others_state*)

Compute Overhauser field term on the bath spin in the cluster from all other spins, not included in the cluster.

Parameters

- **ivec** (*ndarray with shape (3, n, n)*) – Spin vector of the bath spin in the full Hilbert space of the cluster.
- **position** (*ndarray with shape (3,)*) – Position of the bath spin.
- **gyro** (*float*) – Gyromagnetic ratio of the bath spin.
- **other_gyros** (*ndarray with shape (m,)*) – Array of the gyromagnetic ratios of the bath spins, not included in the cluster.
- **others_position** (*ndarray with shape (m, 3)*) – Array of the positions of the bath spins, not included in the cluster.
- **others_state** (*ndarray with shape (m,) or (m, 3)*) – Array of I_z projections for each bath spin outside of the given cluster.

Returns
Bath spin Overhauser term.

Return type
ndarray with shape (n, n)

overhauser_from_tensors(*vec*, *tensors*, *projected_state*)

Compute Overhauser field from array of tensors.

Parameters

- **vec** (*ndarray with shape (3, n, n)*) – Spin vector of the bath spin in the full Hilbert space of the cluster.
- **tensors** (*ndarray with shape (N, 3, 3)*) – Array of interaction tensors.
- **projected_state** (*ndarray with shape (N,)*) – Array of I_z projections of the spins outside of the given cluster..

Returns
Bath spin Overhauser term.

Return type
ndarray with shape (n, n)

`projected_addition`(*vectors*, *bath*, *center*, *state*)

Compute the first order addition of the interactions with the cental spin to the cluster Hamiltonian.

Parameters

- **vectors** (*array-like*) – Array of expanded spin vectors, each with shape (3, n, n).
- **bath** (BathArray) – Array of bath spins.
- **center** (CenterArray) – Array of central spins.
- **state** (*str, bool, or array-like*) – Identificator of the qubit spin. `'alpha'` or `True` for 0 state, `'beta'` of `False` for 1 state.

Returns
Addition to the Hamiltonian.

Return type
ndarray with shape (n, n)

`center_external_addition`(*vectors*, *cluster*, *outer_spin*, *outer_state*)

Compute the first order addition of the interactions between central spin and external bath spins to the cluster Hamiltonian.

Parameters

- **vectors** (*array-like*) – Array of expanded spin vectors, each with shape (3, n, n).
- **cluster** (BathArray) – Array of cluster spins.
- **outer_spin** (*BathArray with shape (o,)*) – Array of the spins outside the cluster.
- **outer_state** (*ndarray with shape (o,)*) – Array of the S_z projections of the external bath spins.

Returns
Addition to the Hamiltonian.

Return type
ndarray with shape (n, n)

`bath_external_point_dipole`(*vectors*, *cluster*, *outer_spin*, *outer_state*)

Compute the first order addition of the point-dipole interactions between cluster spins and external bath spins to the cluster Hamiltonian.

Parameters

- **vectors** (*array-like*) – Array of expanded spin vectors, each with shape (3, n, n).
- **cluster** (BathArray) – Array of cluster spins.
- **outer_spin** (*BathArray with shape (o,)*) – Array of the spins outside the cluster.
- **outer_state** (*ndarray with shape (o,)*) – Array of the S_z projections of the external bath spins.

Returns
Addition to the Hamiltonian.

Return type
ndarray with shape (n, n)

external_spins_field(*vectors*, *indexes*, *bath*, *projected_state*)

Compute the first order addition of the point-dipole interactions between cluster spins and external bath spins to the cluster Hamiltonian.

Parameters

- **vectors** (*array-like*) – Array of expanded spin vectors, each with shape (3, n, n).
- **indexes** (*ndarray with shape (n,)*) – Array of indexes of bath spins inside the given cluster.
- **bath** (*BathArray with shape (N,)*) – Array of all bath spins.
- **projected_state** (*ndarray with shape (N,)*) – Array of the S_z projections of all bath spins.

Returns

Addition to the Hamiltonian.

Return type

ndarray with shape (n, n)

CHAPTER

ELEVEN

UTILITY FUNCTIONS

Here are the various functions used throughout the **PyCCE** code. There is no real structure in this section.

11.1 InteractionMap

`class InteractionMap`(*rows=None*, *columns=None*, *tensors=None*)

Dict-like object containing information about tensor interactions between two spins.

Each key is a tuple of two spin indexes.

Parameters

- **rows** (*array-like with shape (n,)*) – Indexes of the bath spins, appearing on the left in the pairwise interaction.
- **columns** (*array-like with shape (n,)*) – Indexes of the bath spins, appearing on the right in the pairwise interaction.
- **tensors** (*array-like with shape (n, 3, 3)*) – Tensors of pairwise interactions between two spins with the indexes in `rows` and `columns`.

`mapping`

Actual dictionary storing the data.

Type
dict

`property indexes`

Array with the indexes of pairs of spins, for which the tensors are stored.

Type
ndarray with shape (n, 2)

`shift`(*start*, *inplace=True*)

Add an offset `start` to the indexes. If `inplace` is False, returns the copy of InteractionMap.

Parameters

- **start** (*int*) – Offset in indexes.
- **inplace** (*bool*) – If True, makes changes inplace. Otherwise returns copy of the map.

Returns
Map with shifted indexes.

Return type
InteractionMap

keys() → a set-like object providing a view on D's keys

items() → a set-like object providing a view on D's items

subspace(*array*)

Get new InteractionMap with indexes readressed from array. Within the subspace indexes are renumbered.

Examples

The subspace of [3,4,7] indexes will contain InteractionMap only within [3,4,7] elements with new indexes [0, 1, 2].

```
>>> import numpy as np
>>> im = InteractionMap()
>>> im[0, 3] = np.eye(3)
>>> im[3, 7] = np.ones(3)
>>> for k in im: print(k, '\n', im[k],)
(0, 3)
[[1. 0. 0.]
 [0. 1. 0.]
 [0. 0. 1.]]
(3, 7)
 [[1. 1. 1.]
  [1. 1. 1.]
  [1. 1. 1.]]
>>> array = [3, 4, 7]
>>> sim = im.subspace(array)
>>> for k in sim: print(k, '\n', sim[k])
(0, 2)
[[1. 1. 1.]
 [1. 1. 1.]
 [1. 1. 1.]]
```

Parameters

array (*ndarray*) – Either bool array containing True for elements within the subspace or array of indexes presented in the subspace.

Returns

The map for the subspace.

Return type

InteractionMap

classmethod from_dict(*dictionary*, *presorted=False*)

Generate InteractionMap from the dictionary.

Parameters

- **dictionary** (*dict*) – Dictionary with tensors.
- **presorted** (*bool*) – If true, assumes that the keys in the dictionary were already presorted.

Returns

New instance generated from the dictionary.

Return type

InteractionMap

11.2 Noise Filter Functions

Module with helper functions to obtain CPMG coherence from the noise autocorrelation function.

filterfunc(*ts*, *tau*, *npulses*)

Time-domain filter function for the given CPMG sequence.

Parameters

- **ts** (*ndarray with shape (n,)*) – Time points at which filter function will be computed.
- **tau** (*float*) – Delay between pulses.
- **npulses** (*int*) – Number of pulses in CPMG sequence.

Returns
Filter function for the given CPMG sequence.

Return type
ndarray with shape (n,)

gaussian_phase(*timespace*, *corr*, *npulses*, *units='khz'*)

Compute average random phase squared assuming Gaussian noise.

Parameters

- **timespace** (*ndarray with shape (n,)*) – Time points at which correlation function was computed.
- **corr** (*ndarray with shape (n,)*) – Noise autocorrelation function.
- **npulses** (*int*) – Number of pulses in CPMG sequence.
- **units** (*str*) – If units contain frequency or angular frequency ('rad' in `units`).

Returns
Random phase accumulated by the qubit.

Return type
ndarray with shape (n,)

11.3 Spin matrix generators

class SpinMatrix(*s*)

Class containing the spin matrices in Sz basis.

Parameters
s (*float*) – Total spin.

class MatrixDict(**spins*)

Class for storing the SpinMatrix objects.

keys() → a set-like object providing a view on D's keys

stevo(*sm*, *k*, *q*)

Stevens operators (from I.D. Ryabov, Journal of Magnetic Resonance 140, 141–145 (1999)).

Parameters

- **sm** (SpinMatrix) – Spin matrices of the given spin.

- **k** (*int*) – k index of the Stevens operator.
- **q** (*int*) – q index of the Stevens operator.

Returns
Stevens operator representation in S_z basis.

Return type
ndarray with shape (n, n)

dimensions_spinvectors(*bath=None*, *central_spin=None*)

Generate two arrays, containing dimensions of the spins in the cluster and the vectors with spin matrices.

Parameters

- **bath** (*BathArray with shape (n,)*) – Array of the n spins within cluster.
- **central_spin** (*CenterArray, optional*) – If provided, include dimensions of the central spins.

Returns

tuple containing:

- **ndarray with shape (n,)**: Array with dimensions for each spin.
- **list**: List with vectors of spin matrices for each spin in the cluster (Including central spin if `central_spin` is not None). Each with shape (3, N, N) where `N = prod(dimensions)`.

Return type
tuple

vecs_from_dims(*dimensions*)

Generate ndarray of spin vectors, given the array of spin dimensions.

Parameters
dimensions (*ndarray with shape (n,)*) – Dimensions of spins.

Returns
Array of spin vectors in full Hilbert space.

Return type
ndarray with shape (n, 3, X, X)

spinvec(*j*, *dimensions*)

Generate single spin vector, given the index and dimensions of all spins in the cluster.

Parameters

- **j** (*int*) – Index of the spin.
- **dimensions** (*ndarray with shape (n,)*) – Dimensions of spins.

Returns
Spin vector of j-sth spin in full Hilbert space.

Return type
ndarray with shape (3, X, X)

numba_gen_sm(*dim*)

Numba-friendly spin matrix. :param dim: dimensions of the spin marix. :type dim: int

Return type
ndarray

11.4 Other

rotmatrix(*initial_vector*, *final_vector*)

Generate 3D rotation matrix which applied on initial vector will produce vector, aligned with final vector.

Examples

```
>>> R = rotmatrix([0,0,1], [1,1,1])
>>> R @ np.array([0,0,1])
array([0.577, 0.577, 0.577])
```

Parameters

- **initial_vector** (*ndarray with shape(3,)*) – Initial vector.
- **final_vector** (*ndarray with shape (3,)*) – Final vector.

Returns
Rotation matrix.

Return type
ndarray with shape (3, 3)

expand(*matrix*, *i*, *dim*)

Expand matrix M from it's own dimensions to the total Hilbert space.

Parameters

- **matrix** (*ndarray with shape (dim[i], dim[i])*) – Inital matrix.
- **i** (*int*) – Index of the spin dimensions in `dim` parameter.
- **dim** (*ndarray*) – Array pf dimensions of all spins present in the cluster.

Returns
Expanded matrix.

Return type
ndarray with shape (prod(dim), prod(dim))

partial_trace(*dmarray*, *dimensions*, *sel*)

Compute partial trace of the operator (or array of operators).

Parameters

- **dmarray** (*ndarray with shape (N, N) or (m, N, N)*) –
- **dimensions** (*array-like*) – Array of all dimensions of the system.
- **sel** (*int or array-like*) – Index or indexes of dimensions to keep.

Returns
Partially traced operator.

Return type
ndarray with shape (n, n) or (m, n, n)

partial_inner_product(*avec*, *total*, *dimensions*, *index=-1*)

Returns partial inner product $b = a\psi$, where a provided by `avec` contains degrees of freedom to be "traced out" and ψ provided by `total` is the total statevector.

Parameters

- **avec** (*ndarray with shape (a,)*) –
- **total** (*ndarray with shape (a*b,)*) –
- **dimensions** (*ndarray with shape (n,)*) –
- **()** (*index*) –

Returns:

shorten_dimensions(*dimensions*, *central_number*)

Combine the dimensions, corresponding to the central spins.

Parameters

- **dimensions** (*ndarray with shape (n,)*) – Array of the dimensions of the spins in the cluster.
- **central_number** (*int*) – Number of central spins.

Returns
Array of the shortened dimensions;

Return type
ndarray with shape (n - central_number)

outer(*s1*, *s2*)

Outer product of two complex vectors $s_1 ra s_2$.

Parameters

- **s1** (*ndarray with shape (n,)*) – First vector.
- **s2** (*ndarray with shape (m,)*) – Second vector.

Returns
Outer product.

Return type
ndarray with shape (n, m)

tensor_vdot(*tensor*, *ivec*)

Compute product of the tensor and spin vector.

Parameters

- **tensor** (*ndarray with shape (3, 3)*) – Tensor in real space.
- **ivec** (*ndarray with shape (3, n, n)*) – Spin vector.

Returns
Right-side tensor vector product Tv.

Return type
ndarray with shape (3, n, n)

vvdot(*vec_1*, *vec_2*)

Compute product of two spin vectors.

Parameters

- **vec_1** (*ndarray with shape (3, N, N)*) – First spin vector.
- **vec_2** (*ndarray with shape (3, N, N)*) – Second spin vector.

Returns
Product of two vectors.

Return type
ndarray with shape (N, N)

rotate_tensor(*tensor*, *rotation=None*, *style='col'*)

Rootate tensor in real space, given rotation matrix.

Parameters

- **tensor** (*ndarray with shape (3, 3)*) – Tensor to be rotated.
- **rotation** (*ndarray with shape (3, 3)*) – Rotation matrix.
- **style** (*str*) – Can be 'row' or 'col'. Determines how rotation matrix is initialized.

Returns
Rotated tensor.

Return type
ndarray with shape (3, 3)

rotate_coordinates(*xyz*, *rotation=None*, *cell=None*, *style='col'*)

Rootate coordinates in real space, given rotation matrix.

Parameters

- **xyz** (*ndarray with shape (..., 3)*) – Array of coordinates.
- **rotation** (*ndarray with shape (3, 3)*) – Rotation matrix.
- **cell** (*ndarray with shape (3, 3)*) – Cell matrix if coordinates are given in cell coordinates.
- **style** (*str*) – Can be 'row' or 'col'. Determines how rotation matrix and cell matrix are initialized.

Returns
Array of rotated coordinates.

Return type
ndarray with shape (..., 3))

normalize(*vec*)

Normalize vector to 1.

Parameters
vec (*ndarray with shape (n,)*) – Vector to be normalized.

Returns
Normalized vector.

Return type
ndarray with shape (n,)

vec_tensor_vec(*v1*, *tensor*, *v2*)

Compute product v @ T @ v. :param v1: Leftmost expanded spin vector. :type v1: ndarray with shape (3, n, n) :param tensor: 3x3 interaction tensor in real space. :type tensor: ndarray with shape (3, 3) :param v2: Rightmost expanded spin vector. :type v2: ndarray with shape (3, n, n)

Returns
Product vTv.

Return type
ndarray with shape (n, n)

`gen_state_list`(*states*, *dims*)

Generate list of states from S_z projections of the pure states.

Parameters

- **states** (*ndarray with shape (n,)*) – Array of S_z projections.
- **dims** (*ndarray with shape (n,)*) – Array of the dimensions of the spins in the cluster.

Returns
list of state vectors.

Return type
List

`vector_from_s`(*s*, *d*)

Generate vector state from S_z projection.

Parameters

- **s** (*float*) – S_z projection.
- **d** (*int*) – Dimensions of the given spin.

Returns
State vector of a pure state.

Return type
ndarray with shape (d,)

CHAPTER

TWELVE

ES INTERFACE

Each of the interfaces uses subclass of the `DFTCoordinates` class to parse the output.

Note: The interfaces are in beta stage. Please let us know if you encounter any errors.

12.1 Quantum Espresso

class PWCoordinates(*filename*, *pwtype=None*, *to_angstrom=False*)

Coordinates of the system from the PW data of Quantum Espresso. Subclass of the DFTCoordinates.

With initiallization reads either output or input of PW module of QE.

Parameters

- **filename** (*str*) – name of the PW input or output.
- **pwfile** (*str*) – Name of PW input or output file. If the file doesn't have proper extension, parameter pw_type should indicate the type.
- **pwtype** (*str*) – Type of the coord_f. if not listed, will be inferred from extension of pwfile.
- **to_angstrom** (*bool*) – True if automatically convert the units of `cell` and `coordinates` to Angstrom.

parse_output(*filename*, *to_angstrom=False*)

Method to read coordinates of atoms from PW output into the PWCoordinates instance.

Parameters

- **filename** (*str*) – the name of the output file.
- **to_angstrom** (*bool*) – True if automatically convert the units of `cell` and `coordinates` to Angstrom.

Returns
None

parse_input(*filename*, *to_angstrom=False*)

Method to read coordinates of atoms from PW input into the PWCoordinates instance.

Parameters

- **filename** (*str*) – the name of the output file.
- **to_angstrom** (*bool*) – True if automatically convert the units of `cell` and `coordinates` to Angstrom.

cell_from_system(*sdict*)

Function to obtain cell from namelist SYSTEM read from PW input.

Parameters
sdict (*dict*) – Dictinary generated from namelist SYSTEM of PW input.

Returns

Cell is 3x3 matrix with entries:

```
[[a_x b_x c_x]
 [a_y b_y c_y]
 [a_z b_z c_z]],
```

where a, b, c are crystallographic vectors, and x, y, z are their coordinates in the cartesian reference frame.

Return type
ndarray with shape (3,3)

celldms_from_abc(*ibrav*, *abc_list*)

Obtain celldms from ibrav value and a, b, c, cosab, cosac, cosbc parameters.

Using ibrav value and abc parameters from PW input generate celldm array, necessary to construct cell parameters. For details about abc and ibrav values see PW input documentation.

Parameters

- **ibrav** (*int*) – ibrav parameter of PW input.
- **abc_list** (*list*) – List, of 6 parameters: a, b, c, cosab, cosac, cosbc

Returns
list of 6 values, from which cell can be generated.

Return type
celldm (list)

read_gipaw_tensors(*lines*, *keyword=None*, *start=None*, *conversion=1*)

Helper function to read GIPAW tensors from the list of lines.

Parameters

- **lines** (*list of str*) – List of strings contraining lines from the file. Output of open(file).readlines().
- **keyword** (*str*) – Keyword in the line which indicates the beginning of the tensor data block.
- **start** (*int*) – Index of the line which indicates the beginning of the tensor data block.
- **conversion** (*float*) – Conversion factor from GIPAW units to the ones, used in this package.

Returns
Array of tensors.

Return type
ndarray with shape (n, 3, 3)

read_hyperfine(*filename*, *spin=1*)

Function to read hyperfine couplings from GIPAW output.

Parameters

- **filename** (*str*) – Name of the GIPAW hyperfine output.
- **spin** (*float*) – Spin of the central spin. Default 1.

Returns

Tuple containing:

- *ndarray with shape (n,)*: Array of Fermi contact terms.
- *ndarray with shape (n, 3,3)*: Array of spin dipolar hyperfine tensors.

Return type
tuple

read_efg(*filename*)

Function to read electric field gradient tensors from GIPAW output.

Parameters
filename (*str*) – Name of the GIPAW EFG-containing output.

Returns
Array of EFG tensors.

Return type
ndarray with shape (n, 3,3)

read_qe_namelists(*input_string*)

Read Fortran-like namelists from the large string.

Parameters
input_string (*str*) – String representation of the QE input file.

Returns
Dictionary, containing dicts for each namelist found in the input string.

Return type
dict

get_ctype(*lin*)

Get coordinates type from the line of QE input/output.

Parameters
str – Line from QE input/output containing string with coordinates type.

Returns
type of the coordinates.

Return type
str

12.2 ORCA

class ORCACoordinates(*orca_output*)

Coordinates of the system from the ORCA output. Subclass of the DFTCoordinates.

With initialization reads output of the ORCA.

Parameters
orca_output (*str or list of str*) – either name of the output file or list of lines read from that file.

alat

The lattice parameter in angstrom.

Type
float

cell

cell is 3x3 matrix with entries:

$$[[a_x\ b_x\ c_x]$$
$$[a_y\ b_y\ c_y]$$
$$[a_z\ b_z\ c_z]]$$

where a, b, c are crystallographic vectors, and x, y, z are their coordinates in the cartesian reference frame.

Type
ndarray with shape (3, 3)

coordinates

array with the coordinates of atoms in the cell.

Type
ndarray with shape (n, 3)

names

array with the names of atoms in the cell.

Type
ndarray with shape (n,)

cell_units

Units of cell coordinates: 'bohr', 'angstrom', 'alat'.

Type
str

coordinates_units

Units of atom coordinates: 'crystal', 'bohr', 'angstrom', 'alat'.

Type
str

read_output(*orca_output*)

Method to read coordinates of atoms from ORCA output into the ORCACoordinates instance.

Parameters
orca_output (*str or list of str*) – either name of the output file or list of lines read from that file.

12.3 Base class

class DFTCoordinates

Abstract class of a container of the DFT output coordinates.

alat

The lattice parameter in angstrom.

Type
float

`cell`

cell is 3x3 matrix with entries:

$$[[a_x\ b_x\ c_x]$$
$$[a_y\ b_y\ c_y]$$
$$[a_z\ b_z\ c_z]]$$

where a, b, c are crystallographic vectors and x, y, z are their coordinates in the cartesian reference frame.

Type
ndarray with shape (3, 3)

`coordinates`

Array with the coordinates of atoms in the cell.

Type
ndarray with shape (n, 3)

`names`

Array with the names of atoms in the cell.

Type
ndarray with shape (n,)

`cell_units`

Units of cell coordinates: 'bohr', 'angstrom', 'alat'.

Type
str

`coordinates_units`

Units of atom coordinates: 'crystal', 'bohr', 'angstrom', 'alat'.

Type
str

`to_angstrom`(*inplace=False*)

Method to transform cell and coordinates units to angstroms.

Parameters
inplace (*bool*) – if True changes attributes inplace. Otherwise returns copy.

Returns
Instance of the subclass with units of coordinates and cell of Angstroms.

Return type
DFTCoordinates or subclass

`get_angstrom`(*coordinate*, *units*)

Change given coordinates to angstrom.

Parameters

- **coordinates** (*ndarray with shape (n, 3) or (3,)*) – Coordinates to change.
- **units** (*str*) – Initial units of the coordinates.

Returns
Coordinates in angstrom.

Return type
ndarray (n, 3)

change_to_angstrom(*coordinates*, *units*, *alat=None*, *cell=None*)

Change coordinates to angstrom.

Parameters

- **coordinates** (*ndarray with shape (n, 3) or (3,)*) – Coordinates to change.
- **units** (*str*) – Initial units of the coordinates.
- **alat** (*float*) – The lattice parameter in angstrom.
- **cell** (*ndarray with shape (3,3)*) – cell is 3x3 matrix with entries:

$$[[a_x\ b_x\ c_x]$$
$$[a_y\ b_y\ c_y]$$
$$[a_z\ b_z\ c_z]]$$

where a, b, c are crystallographic vectors, and x, y, z are their coordinates in the cartesian reference frame.

Returns
Coordinates in angstrom.

Return type
ndarray with shape (n, 3)

fortran_value(*value*)

Get value from Fortran-type variable.

Parameters
value (*str*) – Value read from Fortran-type input.

Returns
value in Python format.

Return type
value (bool, str, float)

yield_index(*word*, *lines*, *start=0*, *case_sensitive=False*)

Generator which yields indexes of the lines containing specific word.

Parameters

- **word** (*str*) – Word to find in the line.
- **lines** (*list of str*) – List of strings contraining lines from the file. Output of open(file).readlines().
- **start** (*int*) – First index from which to start search.
- **case_sensitive** (*bool*) – If True looks for the exact match. Otherwise the search is case insensitive.

Yields
i (int) – Index of the line containing word.

find_first_index(*word*, *lines*, *start=0*, *case_sensitive=False*)

Function to find first appearance of the index in the list of lines.

Parameters

- **word** (*str*) – Word to find in the line.
- **lines** (*list of str*) – List of strings contraining lines from the file. Output of open(file).readlines().
- **start** (*int*) – First index from which to start search.
- **case_sensitive** (*bool*) – If True looks for the exact match. Otherwise the search is case insensitive.

Returns
Index of the first line from the start containing word.

Return type
i (int)

set_isotopes(*array*, *isotopes=None*, *inplace=True*, *spin_types=None*)

Function to set the most common isotopes for the array containing DFT output. If some other isotope is specified, the A tensors are scaled accordingly.

Parameters

- **array** (BathArray) – Array with DFT spins.
- **isotopes** (*dict*) – Dictionary with chosen isotopes.
- **inplace** (*bool*) – True if change the array inplace.
- **spin_types** (SpinDict) – If provided, allows for custom defined SpinType instances.

Returns
Array with DFT spins with correct isotopes.

Return type
array (*BathArray*)

PyCCE is an open source Python library to simulate the dynamics of a spin qubit interacting with a spin bath using the cluster-correlation expansion (CCE) method.

CHAPTER

THIRTEEN

MAJOR UPDATES

13.1 PyCCE 1.1

- **The PyCCE 1.1 release contains implementation of the master equation-based CCE approaches. Checkout the**
  Dissipative spin bath for examples of the usage.
- Various optimization and bugfixes.

13.2 PyCCE 1.0

The **PyCCE** 1.0 has been released! Main changes from the previous version include:

- **Support for several central spins with the new class `CenterArray`!**
  Check out a tutorial *Multiple central spins* on how to use the new class to study the decoherence of the hybrid qubit or entanglement of dipolarly coupled qubits.
- **Direct definition of the bath spin states with `BathArray.state` attribute.**
  Check out the updated tutorial *NV Center in Diamond* to see how one can use this functionality to study the effect of spin polarization on Hahn-echo signal.
- **Expanded the control over pulse sequences.**
  See documentation for `Pulse` class in *Running the Simulations* for details.
- ***EXPERIMENTAL FEATURE*. Added ability to define your own single particle Hamiltonian.**
  See `BathArray.h` and `Center.h` in *Spin Bath* and *Central spins* respectively for further details.
- Significant overhaul of computational expensive parts of the code with Numba. This makes the first run of **PyCCE** quite slow, but after compilation it should run observably faster.
- Various bug fixes and QoL changes.

This is a major update. If you find any issues ot bugs, please let us know as soon as possible! The **PyCCE** 1.0 has been released! Main changes from the previous version include:

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  Check out the updated tutorial *NV Center in Diamond* to see how one can use this functionality to study the effect of spin polarization on Hahn-echo signal.
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- Various bug fixes and QoL changes.

This is a major update. If you find any issues ot bugs, please let us know as soon as possible!

13.2.1 Known issues

- Numba sometimes raises a warning about non-contiguous arrays. This is a lie.

CHAPTER

FOURTEEN

INSTALLATION

The recommended way to install **PyCCE** is to use **pip**:

```
$ pip install pycce
```

Otherwise you can install **PyCCE** directly using the source code. First copy the repository to the desired folder:

```
$ git clone https://github.com/foxfixfax/pycce.git
```

Then, execute **pip** in the folder containing **setup.py**:

```
$ pip install .
```

or run the python install command:

```
$ python setup.py install
```

CHAPTER

FIFTEEN

REQUIREMENTS

The following modules are required to run **PyCCE**.

- Python (version >= 3.9).
- NumPy (version >= 1.16).
- SciPy (version >= 1.10).
- Numba (version >= 0.56).
- Atomic Simulation Environment (ASE).
- Pandas.

PyCCE inherently supports parallelization with the **mpi4py** package, which requires the installation of MPI. However, for serial implementation the **mpi4py** is not required.

CHAPTER

SIXTEEN

HOW TO CITE

If you make use of **PyCCE** in a scientific publication, please cite the following paper:

> Mykyta Onizhuk and Giulia Galli. "PyCCE: A Python Package for Cluster Correlation Expansion Simulations of Spin Qubit Dynamic" Adv. Theory Simul. 2021, 2100254 https://onlinelibrary.wiley.com/doi/10.1002/adts.202100254

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