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spin coherence with pycce

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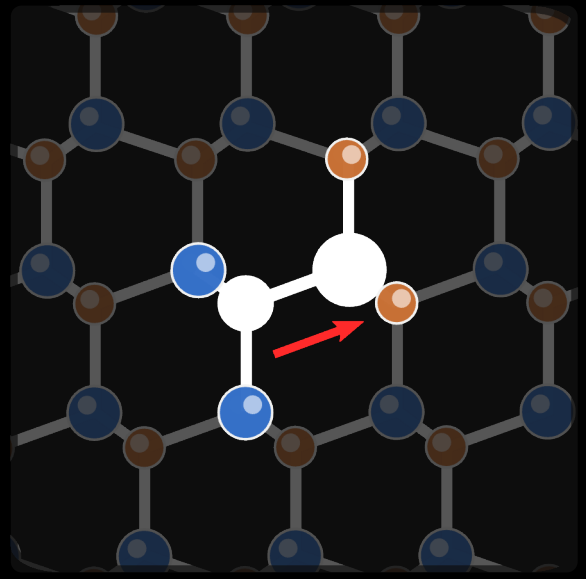
Documentation available at https://pycce.readthedocs.io/

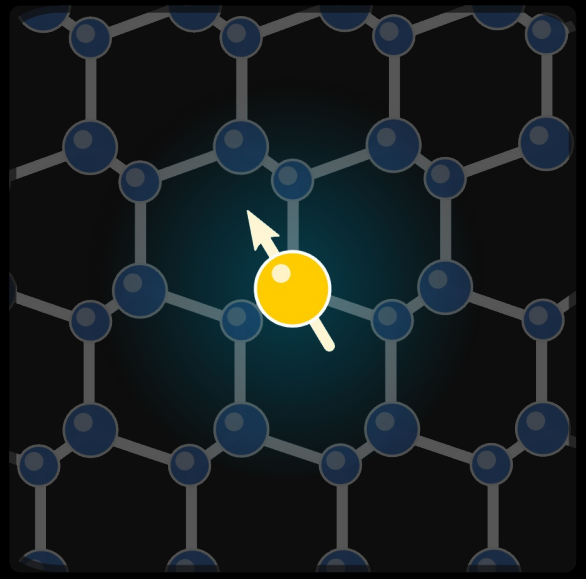
MICCoM

Midwest Integrated Center
for Computational Materials

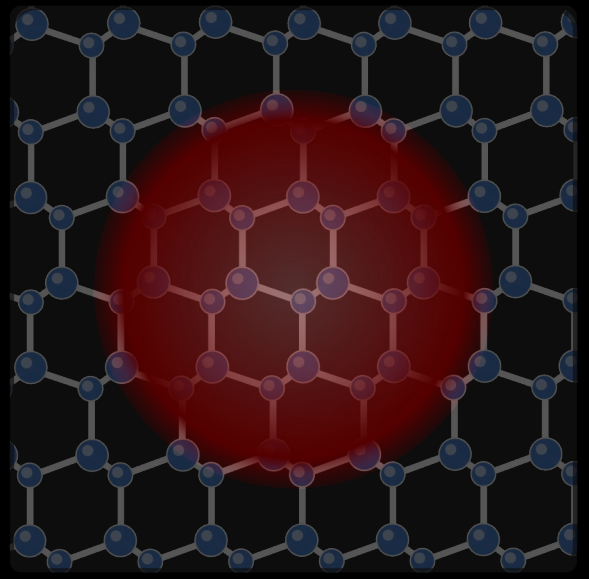
Solid-State Spin is a Leading Platform for Quantum Technologies



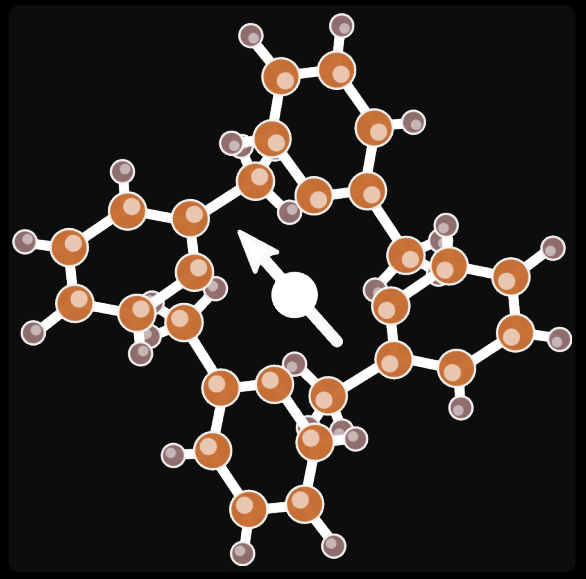
Spin defects



Shallow donors



Quantum dots



Molecular qubits

M Onizhuk and G Galli, Adv. Theory Simul., **4**, 2100254 (2021)

PyCCE – a Python Module for Cluster Correlation Expansion (CCE) Simulations of Spin Dynamics

Includes CCE, gCCE, bath state sampling (nbstates)

To compute coherence, noise correlation

https://pycce.readthedocs.io/en/latest/

Highlights

Object-oriented interface for CCE simulations

Simulator(spin, position=None, alpha=None, beta=None, **kwargs)
The main class for CCE calculations.

Convenient way to generate spin bath

BathArray(shape=None, array=None, **kwargs)
Subclass of ``ndarray`` containing information about the bath spins.

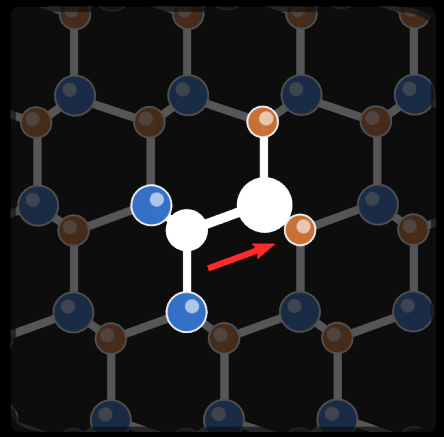
Spin Hamiltonian parameters from ***ab initio*** simulations

read_orca(fname, **kwargs)
Function to read ORCA output containing the hyperfines couplings and EFG tensors.

read_qe(pwfile, hyperfine=None, efg=None, **kwargs)
Function to read PW/GIPAW output from Quantum Espresso into BathArray.

M Onizhuk and G Galli, Adv. Theory Simul., **4**, 2100254 (2021)

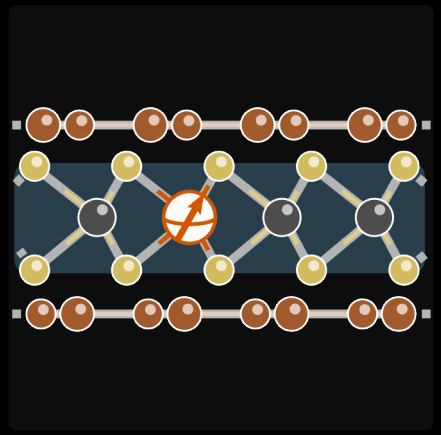
Examples of publications using PyCCE



SiC [1, 2]

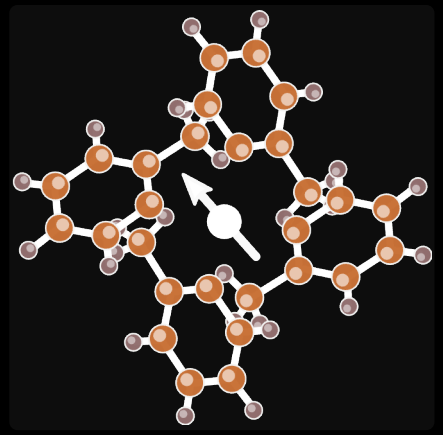
[1] A Bourassa, CP Anderson et al. Nature Materials **19**, 1319-1325 (2020)

[2] M Onizhuk et al. PRX Quantum **2**, 010311 (2021)



Nanomaterials [3]

[3] M Onizhuk, G Galli. APL, **118**, 154003 (2021)



Molecules [4]

[4] SL Bayliss et al. Phys. Rev. X 12, 031028 (2022)

Central Spin Interacting with Dipolar-coupled Spin Bath

System Hamiltonian

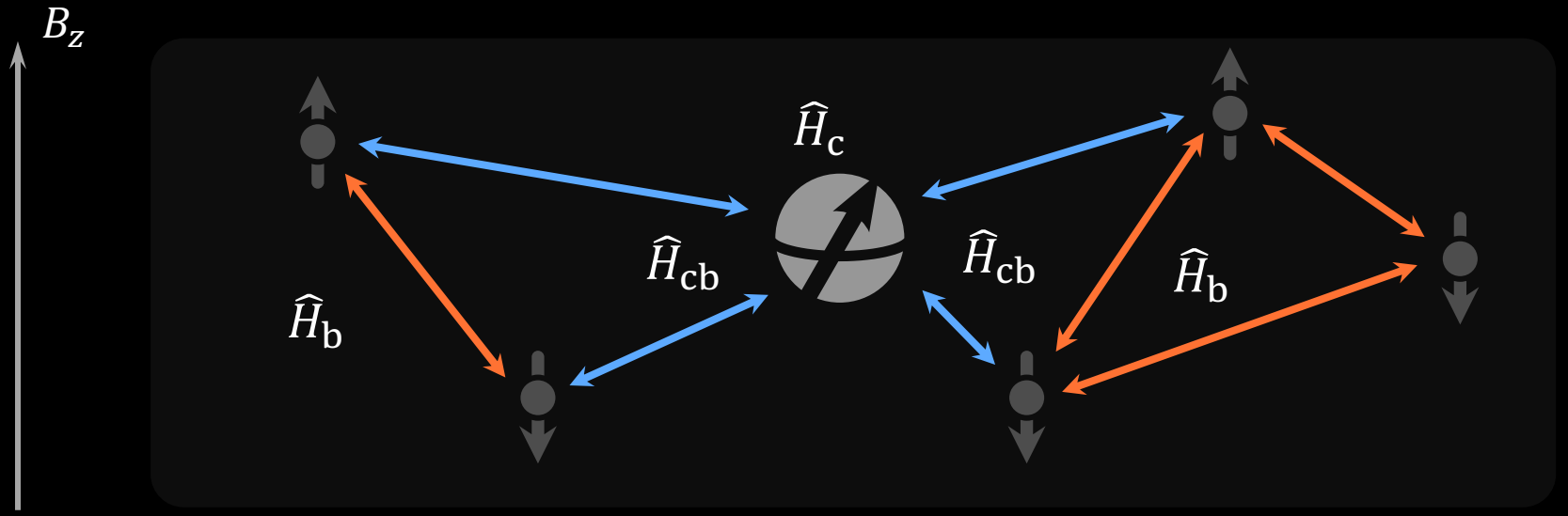
$$\hat{H} = \underbrace{\boldsymbol{SDS} + \gamma_e B_z \hat{S}_z}_{\hat{H}_c} + \underbrace{\sum_i \boldsymbol{SA}\,\boldsymbol{I}_i}_{\hat{H}_{cb}} + \underbrace{\sum_i (\gamma_n B_z \hat{I}_{iz} + \boldsymbol{I}_i \boldsymbol{Q} \boldsymbol{I}_i) + \sum_{i \neq j} \boldsymbol{I}_i \boldsymbol{P} \boldsymbol{I}_j}_{\hat{H}_b}$$

ZFS Zeeman Hyperfine Zeeman Quadrupole Dipole-Dipole

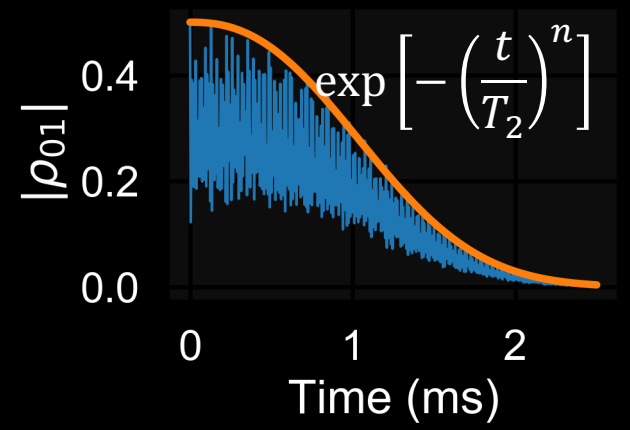
Qubit Density Matrix

$$\begin{bmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{bmatrix}$$

$$\rho_{01} = \langle \hat{S}_{xy} \rangle$$



Coherence dynamics



Projected Hamiltonian

Central Spin-1 Levels

Hamiltonian Projected on Qubit Levels

$$\hat{H} = |0\rangle\hat{H}^{(0)}\langle 0| + |1\rangle\hat{H}^{(1)}\langle 1|$$

Coherence Function – Evolution of the Bath

$$L(t) = \langle 1|\hat{\rho}(t)|0\rangle = \langle \text{Bath}|\, \hat{U}^{(1)\dagger}\hat{U}^{(0)}|\text{Bath}\rangle L(0)$$

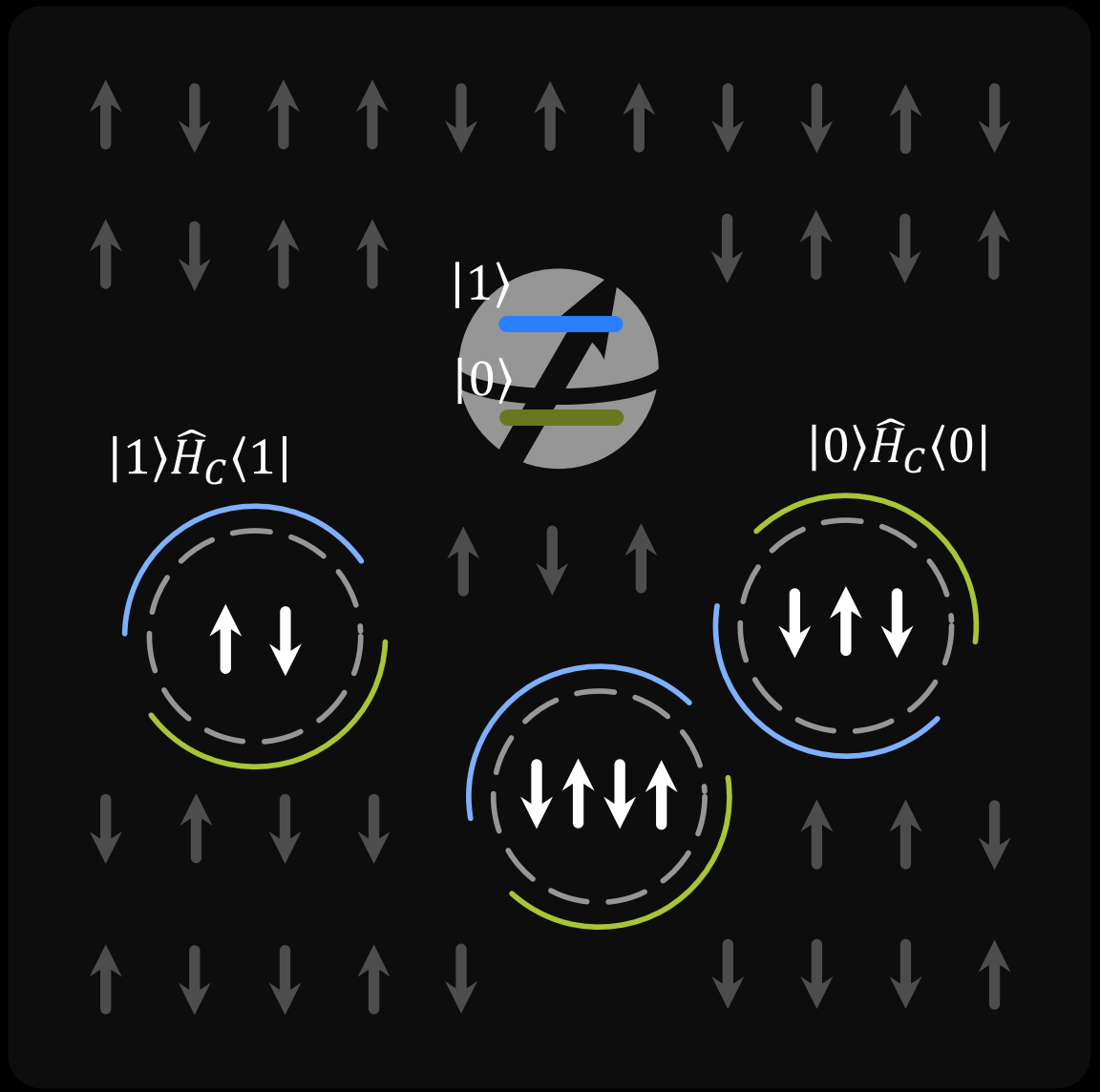
FID

$$\hat{U}^{(0/1)} = e^{-iH^{(0/1)}t}$$

Hahn-Echo

$$\hat{U}^{(0/1)} = e^{-iH^{(1/0)}\tau}\, e^{-iH^{(0/1)}\tau}$$

Cluster Correlation Expansion (CCE)



Coherence Function

CCE2

$$L(t) \approx \prod_{i}^{N} \tilde{L}_{\{i\}} \prod_{i,j}^{N_{\{ij\}}} \tilde{L}_{\{i,j\}} \cdots$$

CCE1

Cluster Contribution

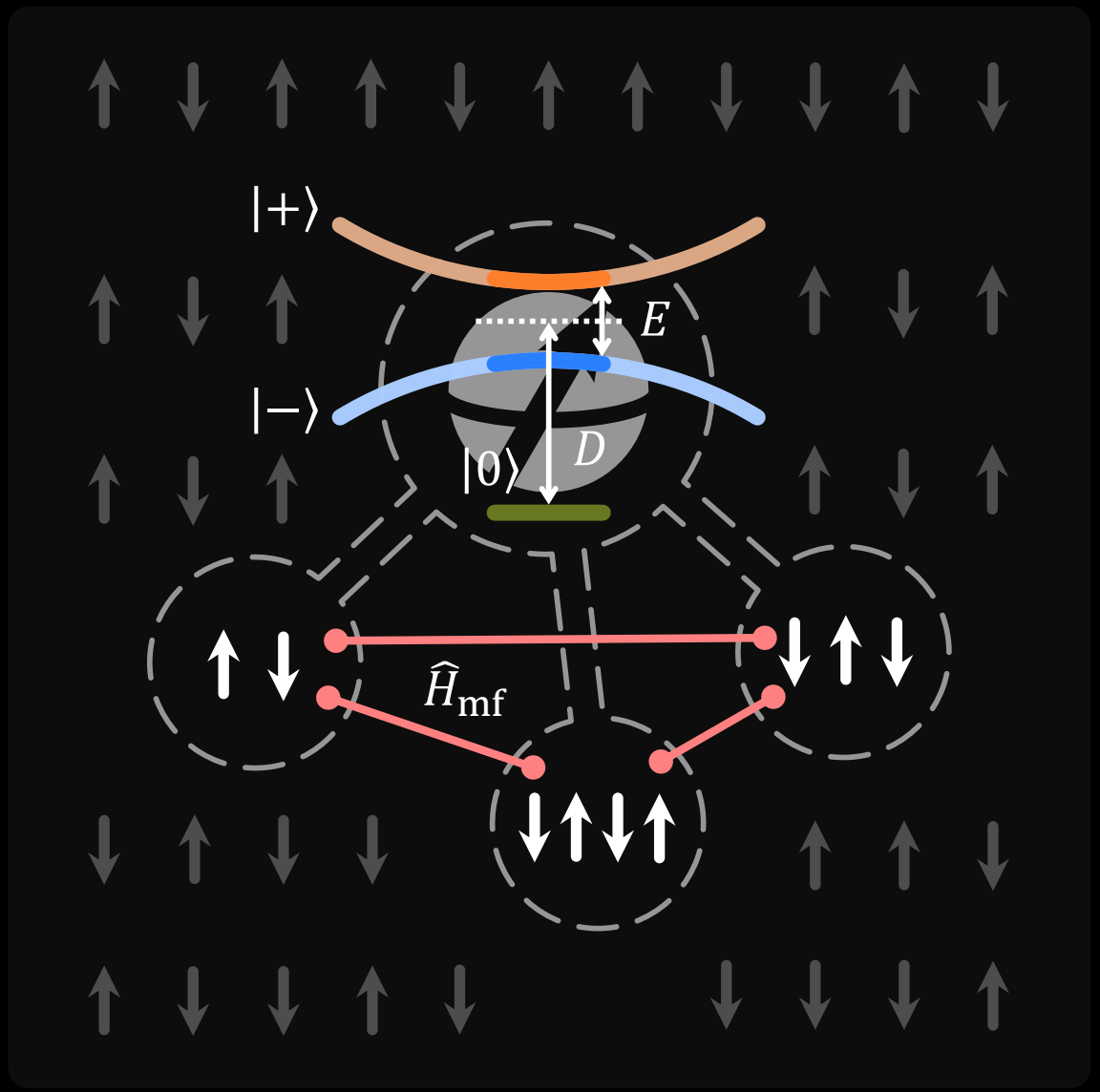
$$\tilde{L}_{\{C\}} = \frac{L_{\{C\}}}{\prod_{C'} \tilde{L}_{\{C' \subset C\}}}$$

Cluster L

$$L_{\{C\}} = \langle \mathrm{C}|\hat{U}_C^{(1)\dagger}\hat{U}_C^{(0)}|\mathrm{C}\rangle$$

W Yang, RB Liu. Phys. Rev. B **78** 085315 (2008)

Generalized CCE



Density Matrix

$$\rho_{ab} = \tilde{\rho}_{ab}^{\{0\}} \prod_{\{i\}} \tilde{\rho}_{ab}^{\{i\}} \prod_{\{i,j\}} \tilde{\rho}_{ab}^{\{ij\}} \cdots$$

Cluster Contribution

$$\tilde{\rho}_{ab}^{\{C\}} = \frac{\langle a|\hat{\rho}^{\{C\}}|b\rangle}{\prod_{C'} \tilde{\rho}_{ab}^{\{C' \subset C\}}}$$

Cluster $\hat{\rho}$

$$\hat{\rho}^{\{C\}}(t) = \hat{U}_C \hat{\rho}^{\{C\}}(0) \hat{U}_C^{\dagger}$$

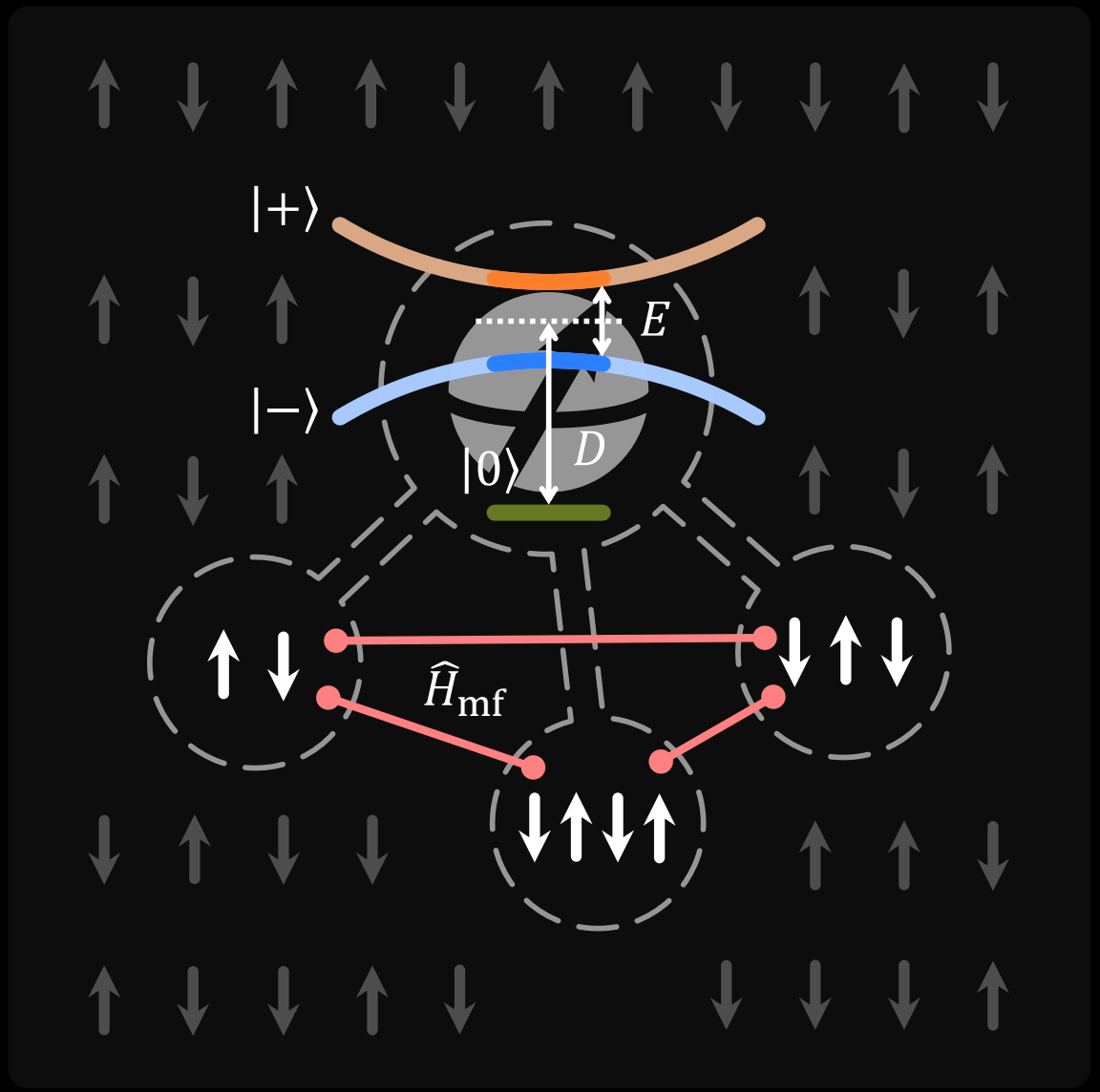
FID

$$\hat{U}_C = e^{-i\hat{H}_C t}$$

Hahn-Echo

$$\hat{U}_C = e^{-i\hat{H}_C \tau}\, e^{-i\sigma_x \frac{\pi}{2}}\, e^{-i\hat{H}_C \tau}$$

Monte-Carlo Sampling of Bath States



Matrix Element for Mixed Bath State

$$\rho_{ab} = \sum_{\mathrm{B}} p_{\mathrm{B}} \rho_{ab}^{\mathrm{B}}$$

$$\mathrm{B} = |\uparrow\downarrow\downarrow \cdots\rangle$$

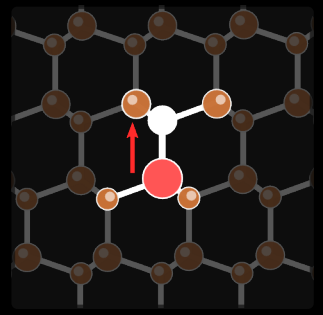
Mean Field Effect of Spins Outside the Clusters

$$\hat{H}_C = \hat{H}_{\mathrm{e}} + \hat{H}_{\mathrm{eb}}^C + \hat{H}_{\mathrm{b}}^C + \hat{H}_{\mathrm{mf}}^C$$

Mean Field Hamiltonian

$$\hat{H}_{\mathrm{mf}}^C = \sum_{i \text{ outside } C} \left[\langle I_z^i \rangle A_{zz} \hat{S}_z + \langle I_z^i \rangle \sum_{j \text{ inside } C} P_{zz} \hat{I}_z^j \right]$$

Examples of using PyCCE module



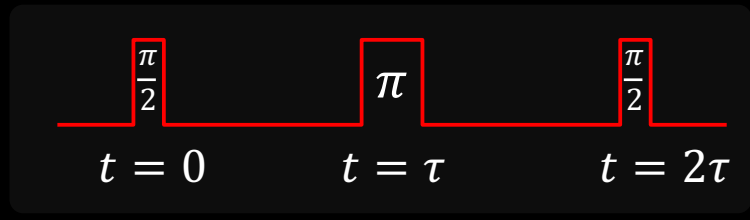
NV^- Center in diamond. Nuclear spin bath

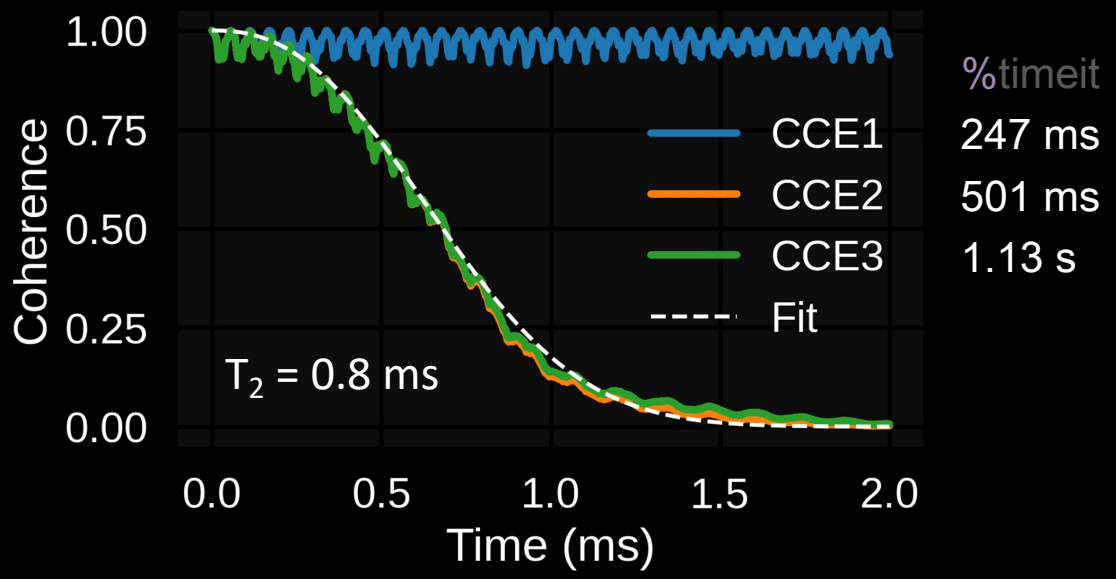
c(^{13}C) = 1.1% nuclear spin bath

Code snippet

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

diamond = pc.bath.BathCell.from_ase(bulk('C', 'diamond', cubic=True)
diamond.zdir = [1, 1, 1]

atoms = diamond.gen_supercell(200, seed=8805)
sim = pc.Simulator(spin=1, D=2.88e6, bath=atoms,
                   alpha=0, beta=1, order=2, r_bath=40, r_dipole=6,
                   pulses=1, magnetic_field=500)

ts = np.linspace(0, 2, 501)
ls = []
for o in range(1, 4):
    sim.order = o
    ls.append(sim.compute(ts).real)
```

Hahn echo signal

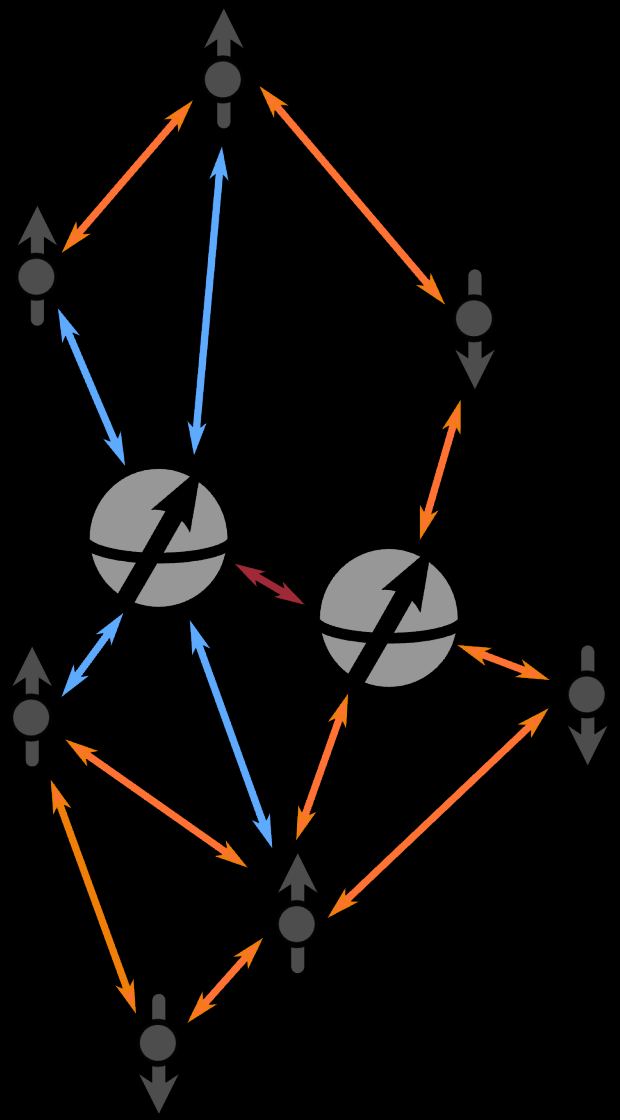




%timeit
247 ms
501 ms
1.13 s

diamond_nv.ipynb

https://colab.research.google.com/github/foxfixfax/PyCCE/blob/master/examples/tutorials/diamond_nv.ipynb



Multiple central spins

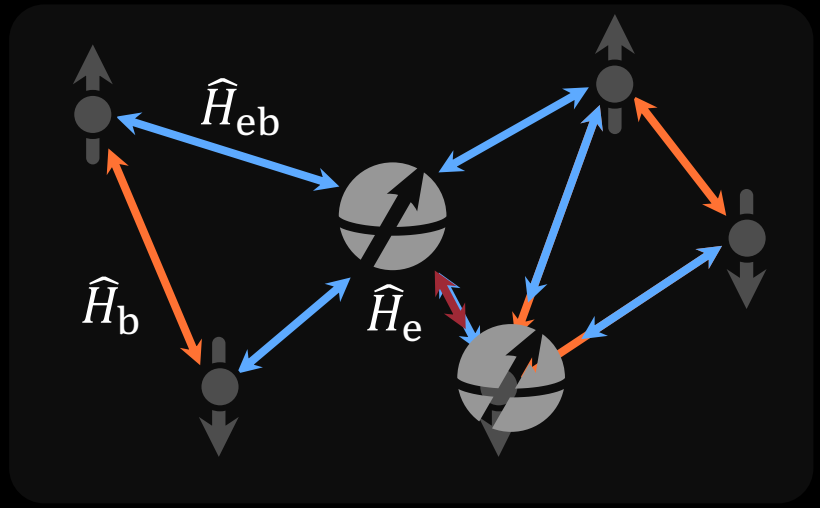
Central Spins Interacting with Dipolar-coupled Spin Bath

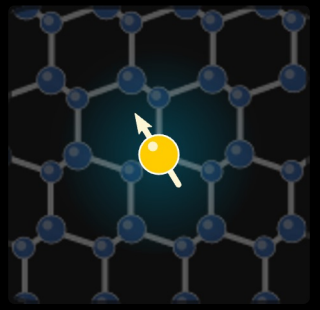
$$\hat{H}_{\mathrm{e}} = \sum_k \boldsymbol{S_k D_k S_k} + \boldsymbol{S_k \gamma_k B} + \sum_{\mathrm{k}<l} \boldsymbol{S_k P S_l}$$

$$\hat{H} = \underbrace{\boldsymbol{SDS} + \boldsymbol{S\gamma_e B}}_{\hat{H}_{\mathrm{e}}} + \underbrace{\sum_i \boldsymbol{SA\, I_i}}_{\hat{H}_{\mathrm{eb}}} + \underbrace{\sum_i \gamma_n B_z \hat{I}_{iz} + \sum_{i<j} \boldsymbol{I_i P I_j}}_{\hat{H}_{\mathrm{b}}}$$

ZFS Zeeman Hyperfine Zeeman Dipole-Dipole

$$\hat{H}_{\mathrm{eb}} = \sum_{i,k} \boldsymbol{S_k A\, I_i}$$





Hybrid register ^{209}Bi donor in Si

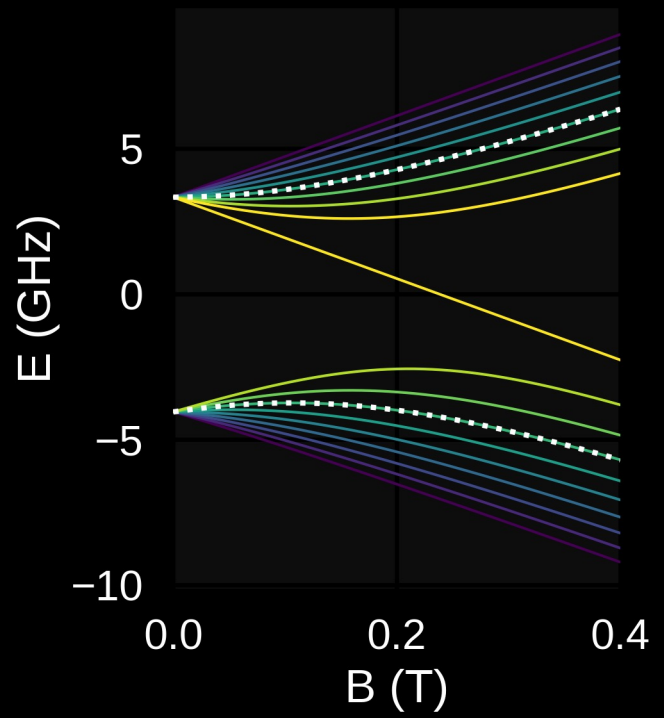
c(^{29}Si) = 4.7% nuclear spin bath

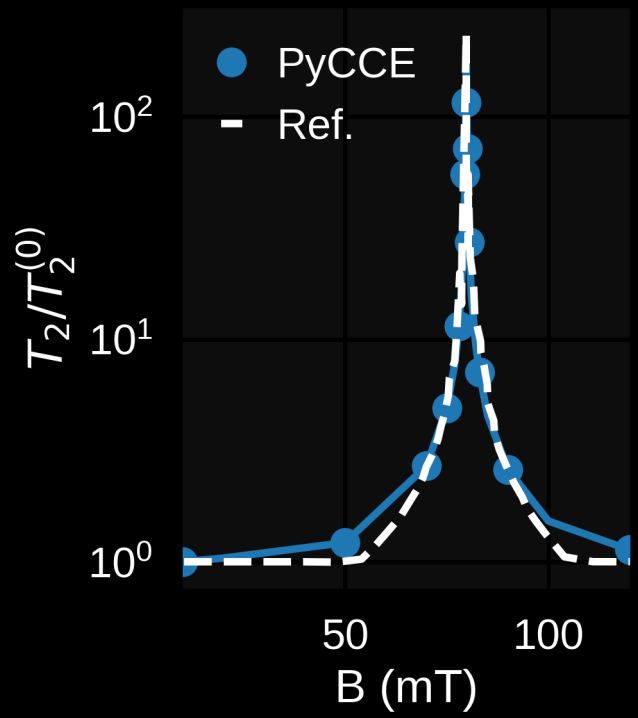
$S = \frac{1}{2}$ 1.47 GHz $I = \frac{9}{2}$

Electron spin Nuclear spin

$$\hat{H}_c = \boldsymbol{S}\gamma_e\mathbf{B} + I\gamma_{Bi}\mathbf{B} + \boldsymbol{SAI}$$

Energy diagram

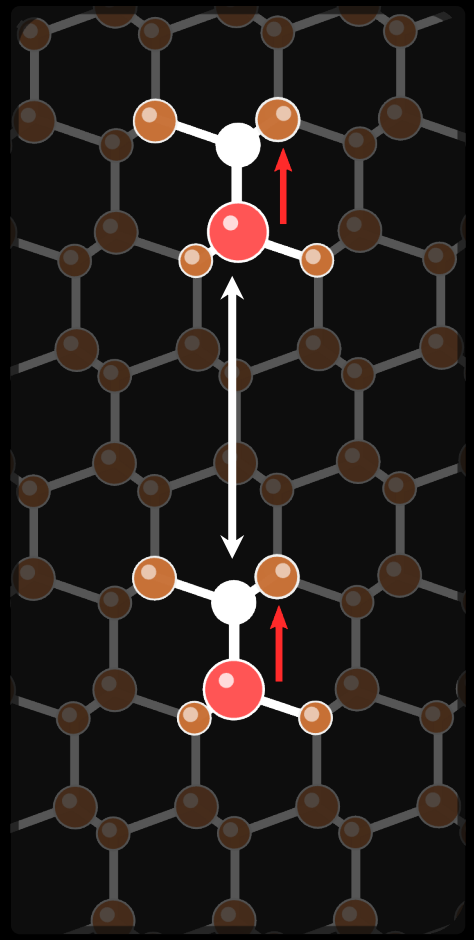




Strong interactions give rise to clock transitions at avoided crossings

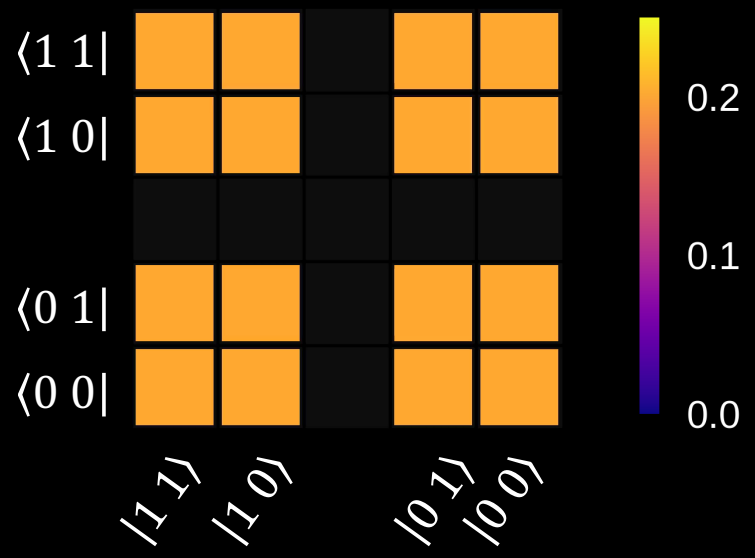
SJ Balian, RB Liu, and TS Monteiro, Phys. Rev. B 91, 245416 (2015)

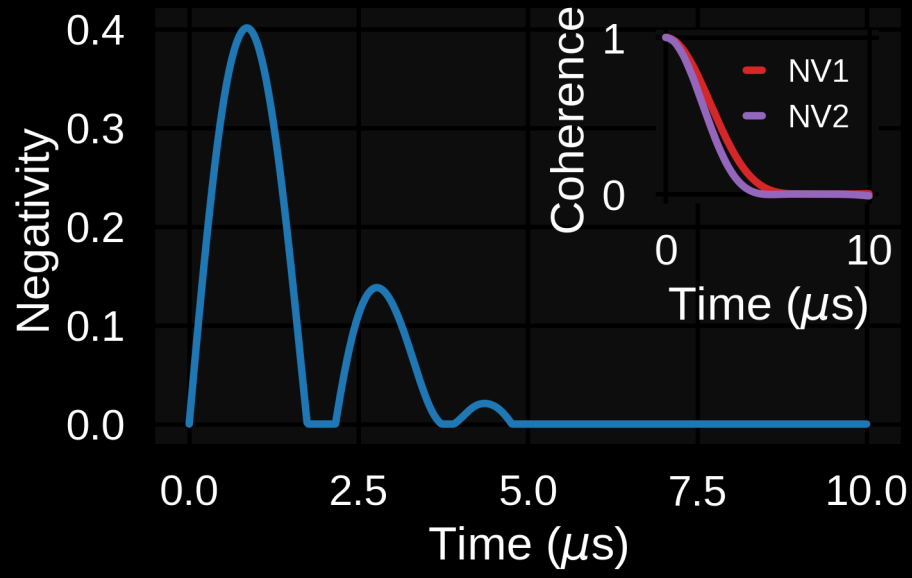
Generation and decay of entanglement between NVs



Initial state of dipolar-coupled NVs

$$|\Psi(0)\rangle = \frac{1}{2}[|0_1\rangle + |1_1\rangle] \otimes [|0_2\rangle + |1_2\rangle]$$





second_spin.ipynb

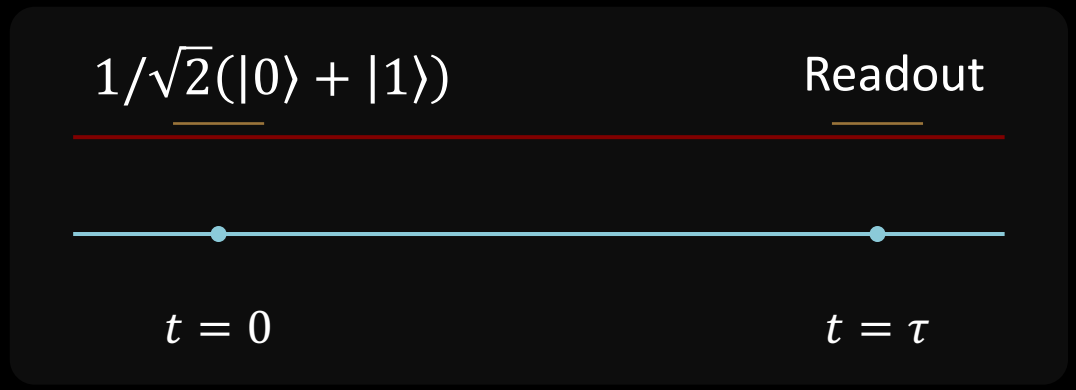
https://colab.research.google.com/github/foxfixfax/PyCCE/blob/master/examples/tutorials/second_spin.ipynb

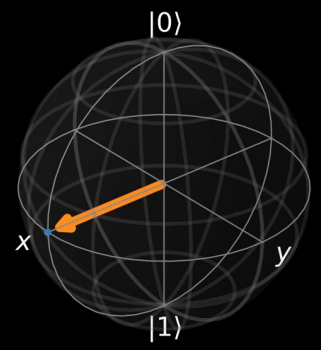
Thank you!

https://pycce.readthedocs.io/en/latest/

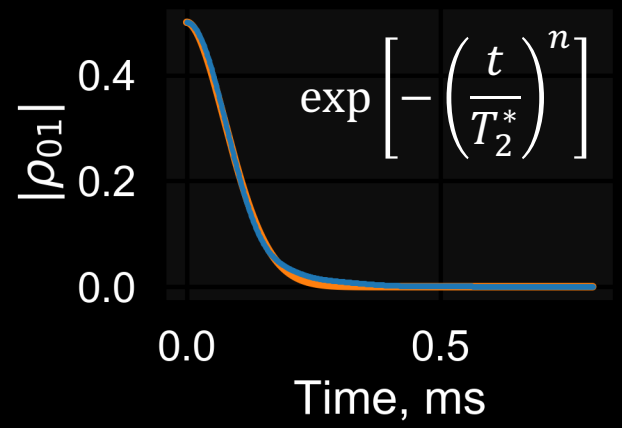
M Onizhuk and G Galli, Adv. Theory Simul., **4**, 2100254 (2021)

Free Induction Decay (FID)

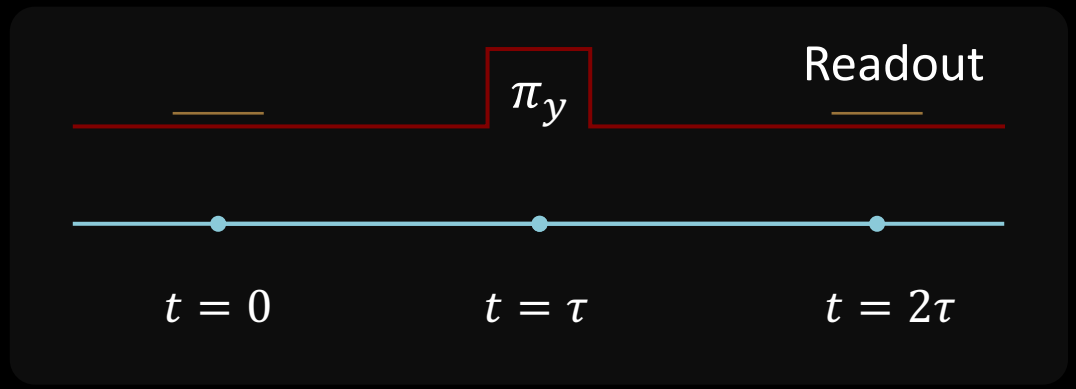


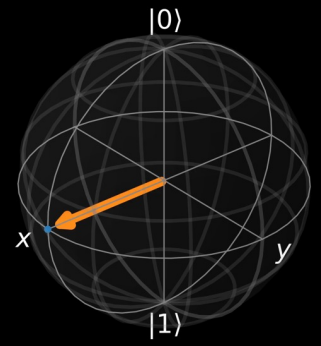


Evolution



Hahn-Echo





π_y-pulse