

Simulation of Spin Systems: QuTiP Demonstration

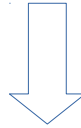
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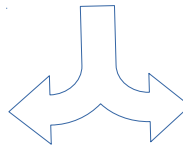
HRI

29th Feb 2016

Simulation of a few-spin quantum systems



QuTiP: Quantum Toolbox in Python



Avian Compass

Diamond NV- Center

QuTiP: Quantum Toolbox in Python

- Based on Python + Scipy framework
- Designed to be a general framework for solving quantum mechanics problems viz. quantum systems with few levels and harmonic oscillators
- Contains large number of functions for performing various quantum operations
- Well tested and open source
- Easy to generate complex Hamiltonians, Liouvillians, wave functions, trace/partial trace etc
- ODE Solver for Schrodinger equation and master equations



QuTiP: Basics

- Quantum states, operators etc. are represented by a data structure called Qobj

- Defining a state $|\psi\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

```
>> psi = Qobj([[1], [0]])
>> print psi
Quantum object: dims = [[2], [1]], shape = [2, 1]
Qobj data =
[[1]
 [0]]
```

- Operations on quantum states $|\psi_{up}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}; |\psi_{down}\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad |\psi\rangle = \frac{|\psi_{up}\rangle + |\psi_{down}\rangle}{\sqrt{2}}$

```
>> psi_up = Qobj([[0], [1]])
>> psi_down = Qobj([[1], [0]])
>> psi = (psi_up + psi_down) / sqrt(2)
>> print psi
Quantum object: dims = [[2], [1]], shape = [2, 1]
Qobj data =
[[ 0.70710678]
 [ 0.70710678]]
```

- Fock state

$$|\psi_{fock}\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\rho_{fock} = |\psi_{fock}\rangle \langle \psi_{fock}|$$

- Tensor product

- Partial trace

```
>> print fock(4, 1)
Quantum object: dims = [[4], [1]], shape = [4, 1]
Qobj data =
[[ 0.]
 [ 1.]
 [ 0.]
 [ 0.]]
>> print fock_dm(4, 1)
Quantum object: dims = [[4], [4]], shape = [4, 4]
Qobj data =
[[ 0.  0.  0.  0.]
 [ 0.  1.  0.  0.]
 [ 0.  0.  0.  0.]
 [ 0.  0.  0.  0.]]

>> rho=tensor([fock_dm(2,0), fock_dm(2,1)])
>> print ptrace(rho,0)
Quantum object: dims = [[2], [2]], shape = [2, 2]
Qobj data =
[[ 1.  0.]
 [ 0.  0.]]
>> print ptrace(rho,1)
Quantum object: dims = [[2], [2]], shape = [2, 2]
Qobj data =
[[ 0.  0.]
 [ 0.  1.]]
```


Hamiltonian: Examples

- Two interacting qubit: $H = \sigma_z^{(1)} + \sigma_z^{(2)} + 0.01\sigma_x^{(1)}\sigma_x^{(2)}$

```
>> sz1 = tensor([sigmaz(), qeye()])
>> sz2 = tensor([qeye(), sigmaz()])
>> sxsx = tensor([sigmax(), sigmax()])
>> H = sz1 + sz2 + 0.1 * sxsx
>> print H
Quantum object: dims = [[2, 2], [2, 2]], shape = [4, 4]
Qobj data =
[[ 2.  0.  0.  0.1]
 [ 0.  0.  0.1  0. ]
 [ 0.  0.1  0.  0. ]
 [ 0.1  0.  0. -2. ]]
```

- Qubit coupled to a harmonic oscillator bath: $H = \omega a^\dagger a + \epsilon \sigma_z + g(a^\dagger \sigma^- + a \sigma^+)$

```
>> N = 10; w = 1; eps = 1; g = 0.01
>> a = tensor([destroy(N), qeye(2)])
>> sz = tensor([qeye(N), sigmaz()])
>> sm = tensor([qeye(N), sigmam()])
>> H = w * a.dag() * a + eps * sz + g * (a.dag() * sm + a * sm.dag())
>> print H
Quantum object: dims = [[10, 2], [10, 2]], shape = [20, 20]
Qobj data =
...
```

Time Evolution: Unitary time evolution

$$H |\psi\rangle = i\hbar \frac{\partial}{\partial t} |\psi\rangle; |\psi(0)\rangle = \psi_0$$

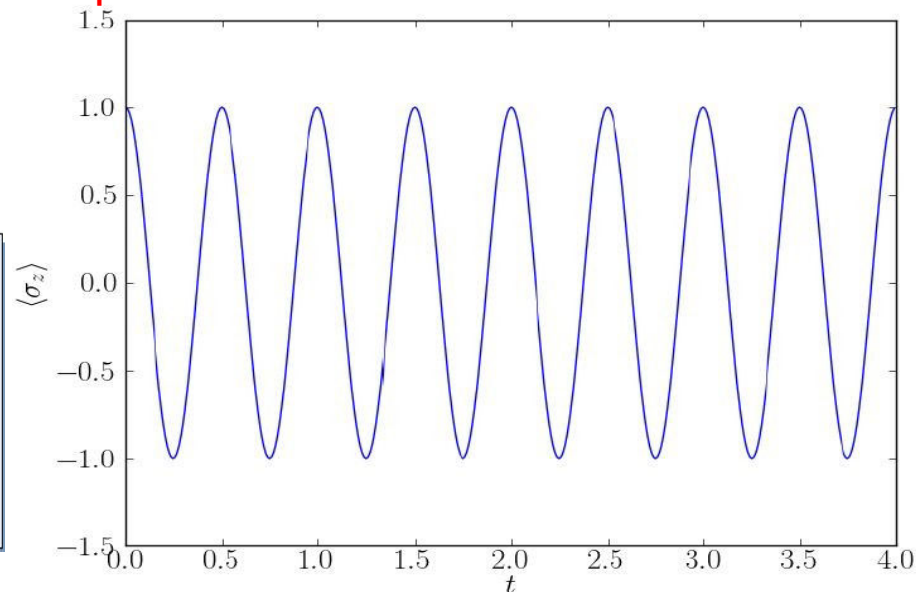
QuTiP: `result = ode_solve(H, psi_0, tlist, [], expt_op_list)`

- H = **Hamiltonian**
- ψ_0 = **initial wave function**
- $tlist$ = **time instants at which result is to be stored**
- $expt_op_list$ = **expectation value of these operator is stored (at specified time)**
- $result$ = **state values stored at time instants specified in $tlist$**

$$\langle A(t) \rangle = \langle \psi(t) | A | \psi(t) \rangle$$

Example:

```
>> H = 2 * pi * sigmax()
>> psi0 = fock(2, 0)           # |0> state
>> tlist = arange(0.0, 4.0, 0.01)
>> expt_sz = ode_solve(H, psi0, tlist, [], [sigmaz()])
>> plot(tlist, expt_sz[0])
>> show()
```



Time Evolution: Master equation

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \Gamma \sum_{i=1}^8 (L_i \rho L_i^\dagger - \frac{1}{2}(L_i^\dagger L_i \rho + \rho L_i^\dagger L_i))$$

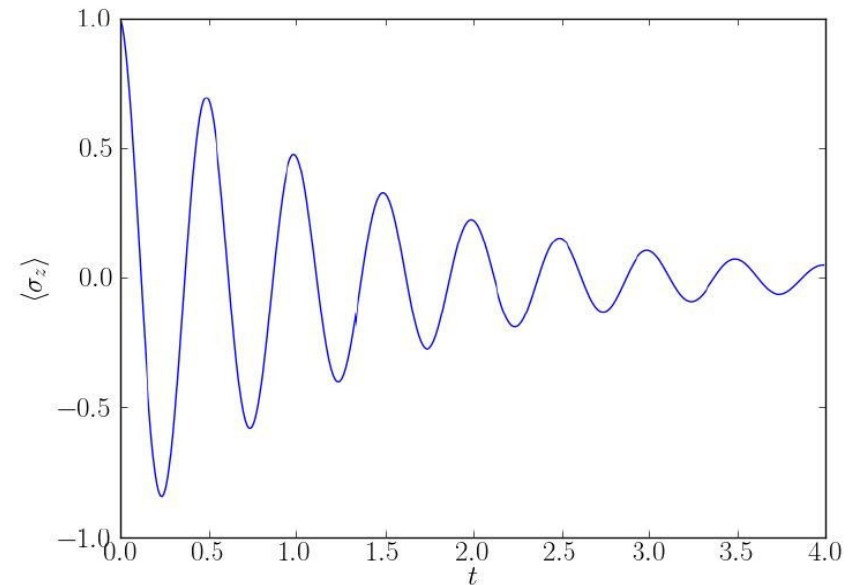
QuTiP: `result = ode_solve(H, psi0, tlist, c_op_list, expt_op_list)`

- H = Hamiltonian
- psi0 = an initial wave function
- tlist = time instants at which result is to be stored
- c_op_list = list of collapse operators
- expt_op_list = expectation value of these operator is stored (at specified time)

Alternatively: `result = mesolve(H, rho0, tlist, c_ops, expt_ops, args={}, options=None)`

Example:

```
>> H = 2 * pi * sigmax()
>> psi0 = fock(2, 0)           # |0> state
>> gamma1 = 1.0
>> c_ops = [sqrt(gamma1) * sigmam()] # relaxation
>> expt_ops = [sigmaz()]
>> tlist = arange(0.0, 4.0, 0.01)
>> expt_sz = ode_solve(H, psi0, tlist, c_ops, expt_ops)
>> plot(tlist, expt_sz[0])
```



QuTiP Demos: Inbuilt Examples

```
Qubit: demos()
```

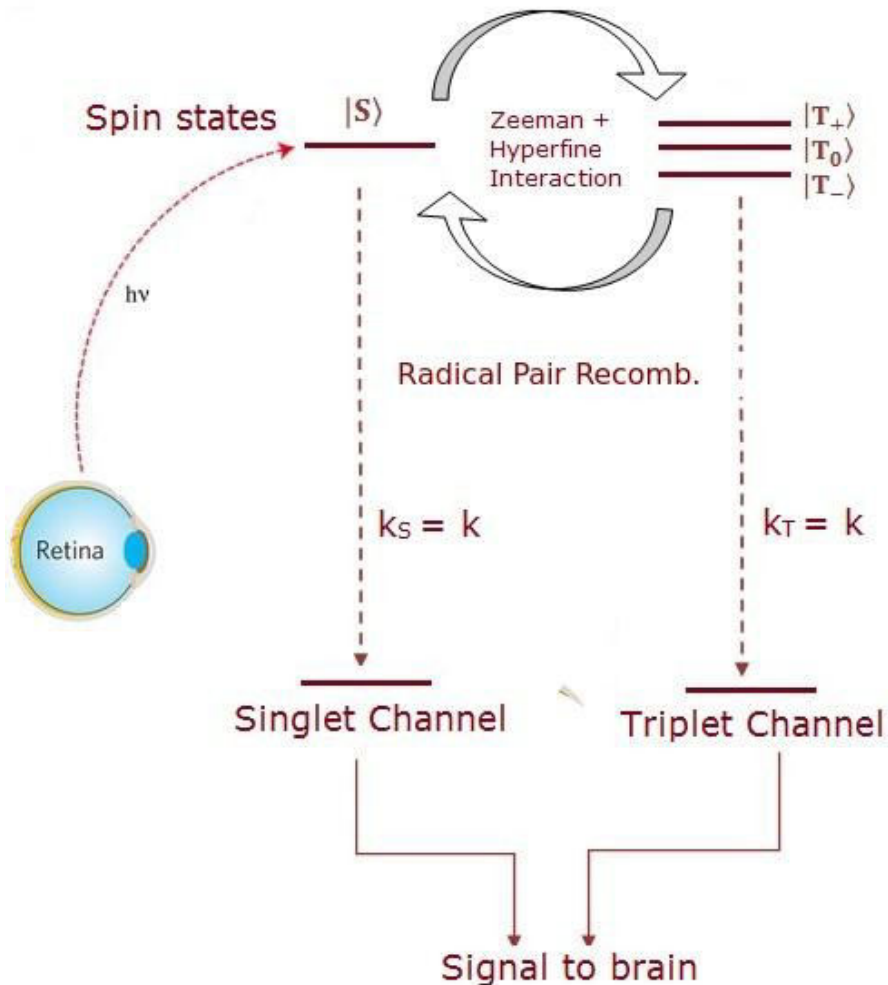
Rabi Oscillations

Bloch Sphere Spin Dynamics

Time Evolution and Dynamics

..... and many more

Avian Compass: RP Spin Dynamics



- Fraction of radical pairs recombining to singlet channel \rightarrow **Singlet Yield**
- Fraction of radical pairs recombining to triplet channel \rightarrow **Triplet Yield**
- Singlet and Triplet yields contain the information about the ambient magnetic field

The Formalism

Lindblad Master Equation:

$$\dot{\rho} = \underbrace{-\frac{i}{\hbar}[H, \rho]}_{\text{Unitary evolution}} + \underbrace{k \sum_{i=1}^8 P_i \rho P_i^\dagger - \frac{1}{2}(P_i^\dagger P_i \rho + \rho P_i^\dagger P_i)}_{\text{Recombination}}.$$

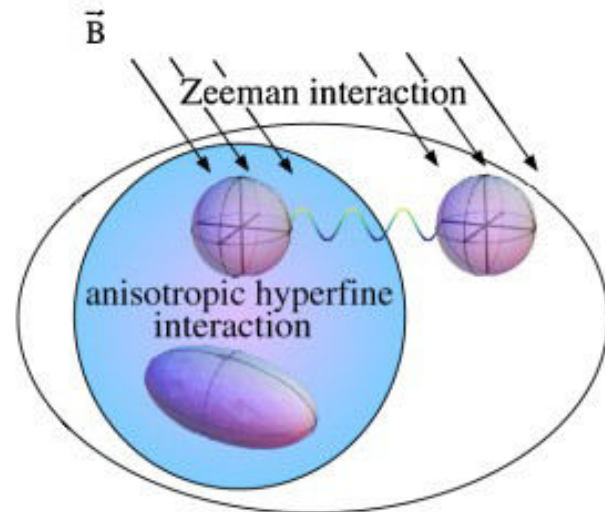
P_i : Recombination to singlet and triplet channels

$$\begin{aligned} P_1 &= |SC\rangle\langle S \uparrow| \\ P_2 &= |TC\rangle\langle T_0 \uparrow| \\ P_3 &= |TC\rangle\langle T_+ \uparrow| \\ P_4 &= |TC\rangle\langle T_- \uparrow| \end{aligned}$$

$$\begin{aligned} P_5 &= |SC\rangle\langle S \downarrow| \\ P_6 &= |TC\rangle\langle T_0 \downarrow| \\ P_7 &= |TC\rangle\langle T_+ \downarrow| \\ P_8 &= |TC\rangle\langle T_- \downarrow| \end{aligned}$$

Hamiltonian

$$H = \underbrace{\gamma \mathbf{B} \cdot (\hat{S}_1 + \hat{S}_2)}_{\text{Zeeman}} + \underbrace{\hat{I} \cdot \mathbf{A} \cdot \hat{S}_2}_{\text{Hyperfine}}$$



$$H = H_{nuc} \otimes H_{e1} \otimes H_{e2}$$

$$H_{hyp} = a_x I_x S_x + a_y I_y S_y + a_z I_z S_z \quad \mathbf{A} = \text{diag}(a_x, a_y, a_z)$$

$$H_{hyp} = a_x(\sigma_x \otimes I \otimes \sigma_x) + a_y(\sigma_y \otimes I \otimes \sigma_y) + a_z(\sigma_z \otimes I \otimes \sigma_z)$$

$$H_{Zeeman} = \gamma(B_x(S_{1x} + S_{2x}) + B_y(S_{1y} + S_{2y}) + B_z(S_{1z} + S_{2z}))$$

$$H_{Zeeman} = \gamma B_x(I \otimes \sigma_x \otimes I + I \otimes I \otimes \sigma_x) + \gamma B_y(I \otimes \sigma_y \otimes I + I \otimes I \otimes \sigma_y) \\ + \gamma B_z(I \otimes \sigma_z \otimes I + I \otimes I \otimes \sigma_z)$$

Density Matrix

- Three spin system (Each spin 1/2): **8 dim Hilbert Space**
- This Hilbert space is extended to 10 dims to account for two **recombination channels**

$$\rho = [\rho_{nuc} \otimes \rho_{elec1} \otimes \rho_{elec2}] + 2 \text{ recomb. channel states}$$

- The matrix elements corresponding to 9th and 10th dimension give the **singlet** and **triplet** yields

Initial State

- Initially, the RP is in singlet state: $|s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$
- Initial state: $\rho(0) = \frac{1}{2}I \otimes (|s\rangle \otimes \langle s|)$

Projection Operator

Define: P_i Projection from singlet and triplet states to recombination channels

$$\begin{aligned}P_1 &= |SC\rangle\langle S \uparrow| \\P_2 &= |TC\rangle\langle T_0 \uparrow| \\P_3 &= |TC\rangle\langle T_+ \uparrow| \\P_4 &= |TC\rangle\langle T_- \uparrow|\end{aligned}$$

$$\begin{aligned}P_5 &= |SC\rangle\langle S \downarrow| \\P_6 &= |TC\rangle\langle T_0 \downarrow| \\P_7 &= |TC\rangle\langle T_+ \downarrow| \\P_8 &= |TC\rangle\langle T_- \downarrow|\end{aligned}$$

State Evolution

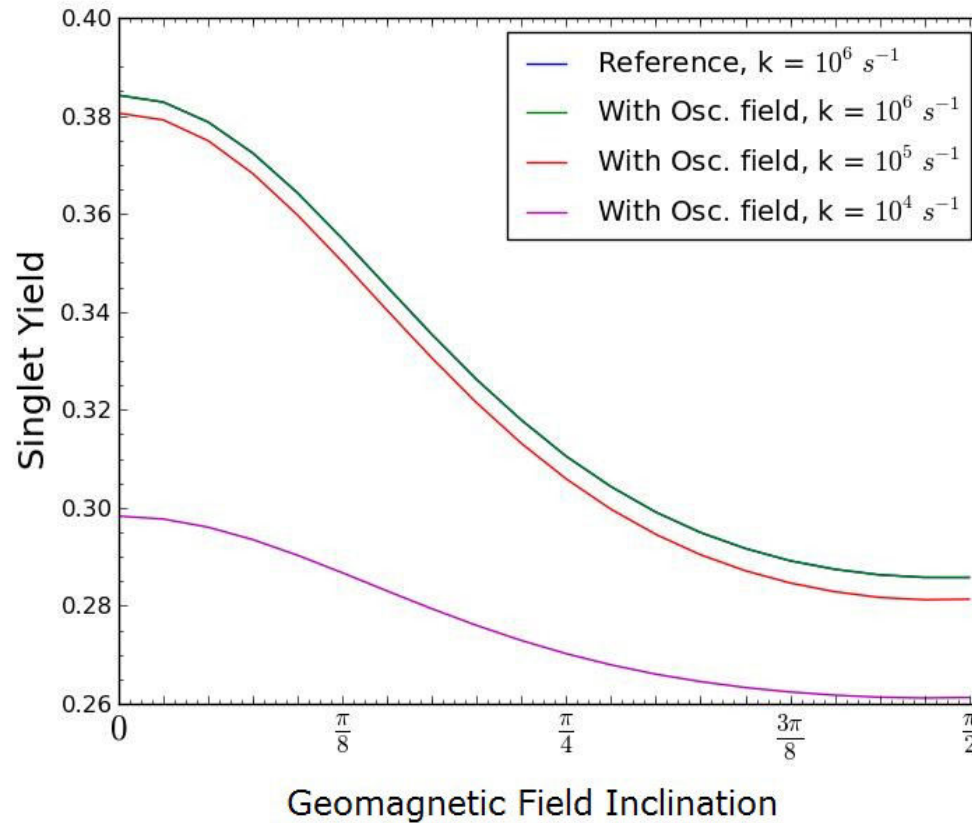
$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + k \sum_{i=1}^8 P_i \rho P_i^\dagger - \frac{1}{2}(P_i^\dagger P_i \rho + \rho P_i^\dagger P_i).$$

- After defining Hamiltonian, initial state and, projection operators this master equation is solved using `mesolve` function.

```
result = mesolve(H, rho0, tlist, c_ops, expt_ops, args={}, options=None)
```

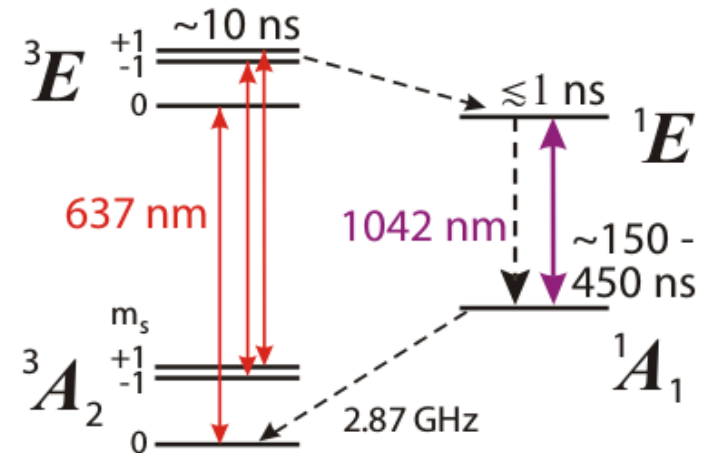
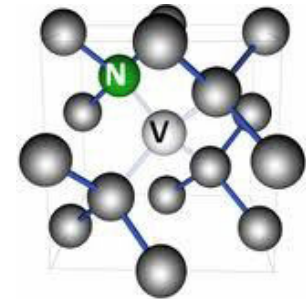
- `result` stores the density matrix at each time instant
- The 9th diagonal element is the **singlet yield** and 10th diagonal element is the **triplet yield** of the reaction
- The singlet and triplet yields are plotted against the magnetic field

Results: Singlet yield vs geomagnetic field



Diamond NV Center – Electronic Structure

- NV-center has triplet ground and excited states with ZFS
- **Optical transitions:** Optical pumping at 637nm
Radiative and non-radiative transitions
- **Spin Dynamics:** Transition between the spin sublevels of a given spin state
- The ground and excited state can evolve under the magnetic field
- Fluctuating magnetic fields dephase the spin state



Ground State and Excited State Hamiltonian

- Ground State Hamiltonian

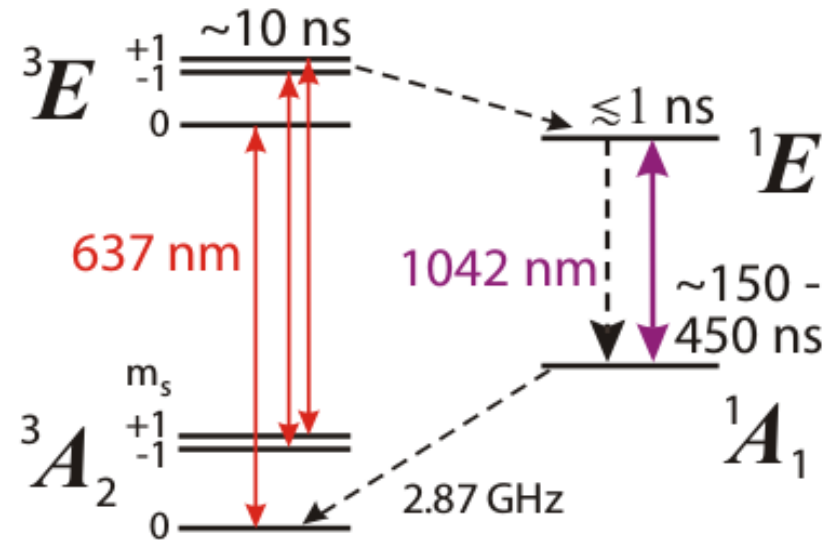
$$\hat{H}_{gs} = D_{gs} \left[\hat{S}_z^2 - S(S + 1)/3 \right] + A_{gs}^{\parallel} \hat{S}_z \hat{I}_z + A_{gs}^{\perp} \left[\hat{S}_x \hat{I}_x + \hat{S}_y \hat{I}_y \right] + P_{gs} \left[\hat{I}_z^2 - I(I + 1)/3 \right]$$

- Excited State Hamiltonian

$$\hat{H}_{es}^{RT} = D_{es}^{\parallel} \left[\hat{S}_z^2 - S(S + 1)/3 \right] + A_{es}^{\parallel} \hat{S}_z \hat{I}_z + A_{es}^{\perp} \left[\hat{S}_x \hat{I}_x + \hat{S}_y \hat{I}_y \right] + P_{es} \left[\hat{I}_z^2 - I(I + 1)/3 \right]$$

Simulation Scheme

- NV center is spin 1 system with spin 1 nucleus
[Two 3 level systems]
- Ground state and excited states evolve under 9 dimensional Hilbert space



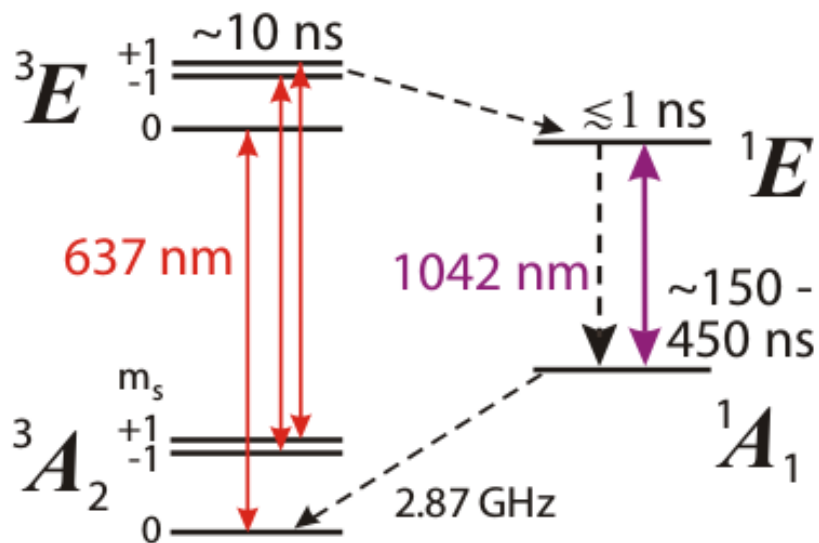
- Total Hamiltonian
$$H = \begin{bmatrix} [H_{gs}] & 0 & 0 \\ 0 & [H_{es}] & 0 \\ 0 & 0 & [SS] \end{bmatrix}$$

$$H_{gs} = 9 \times 9$$

$$H_{es} = 9 \times 9$$

$$SS = 2 \times 2$$

Projection Operators



$$H = \begin{bmatrix} [H_{gs}] & 0 & 0 \\ 0 & [H_{es}] & 0 \\ 0 & 0 & [SS] \end{bmatrix}$$

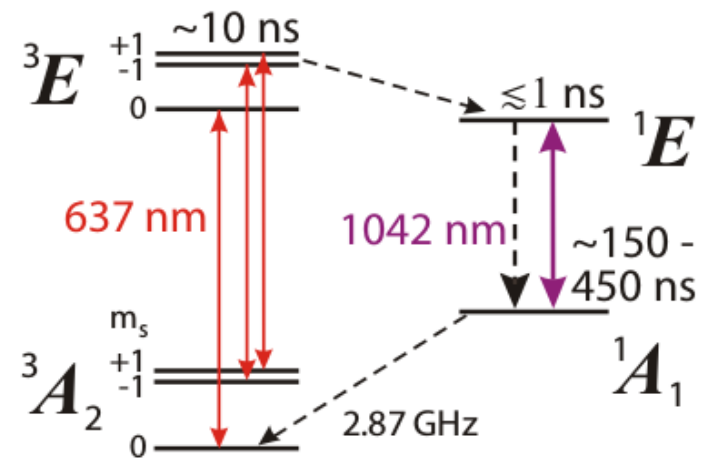
- $P1 = 3E(m_s=+1, m_l=-1) \rightarrow 1E$
- $P2 = 3E(m_s=+1, m_l=0) \rightarrow 1E$
- $P3 = 3E(m_s=+1, m_l=+1) \rightarrow 1E$
- $P4 = 3E(m_s=-1, m_l=-1) \rightarrow 1E$
- $P5 = 3E(m_s=-1, m_l=0) \rightarrow 1E$
- $P6 = 3E(m_s=-1, m_l=+1) \rightarrow 1E$
- $P7 = 1E \rightarrow 1A$
- $P8 = 3E(m_s=0, m_l=-1) \rightarrow 3A(m_s=0, m_l=-1)$
- $P9 = 3E(m_s=0, m_l=0) \rightarrow 3A(m_s=0, m_l=0)$
- $P10 = 3E(m_s=0, m_l=+1) \rightarrow 3A(m_s=0, m_l=+1)$
- $P11 = 3E(m_s=+1, m_l=-1) \rightarrow 3A(m_s=+1, m_l=-1)$
- $P12 = 3E(m_s=+1, m_l=0) \rightarrow 3A(m_s=+1, m_l=0)$
- $P13 = 3E(m_s=+1, m_l=+1) \rightarrow 3A(m_s=+1, m_l=+1)$
- $P14 = 3E(m_s=-1, m_l=-1) \rightarrow 3A(m_s=-1, m_l=-1)$
- $P15 = 3E(m_s=-1, m_l=0) \rightarrow 3A(m_s=-1, m_l=0)$
- $P16 = 3E(m_s=-1, m_l=+1) \rightarrow 3A(m_s=-1, m_l=+1)$

Phenomenological Master Equation

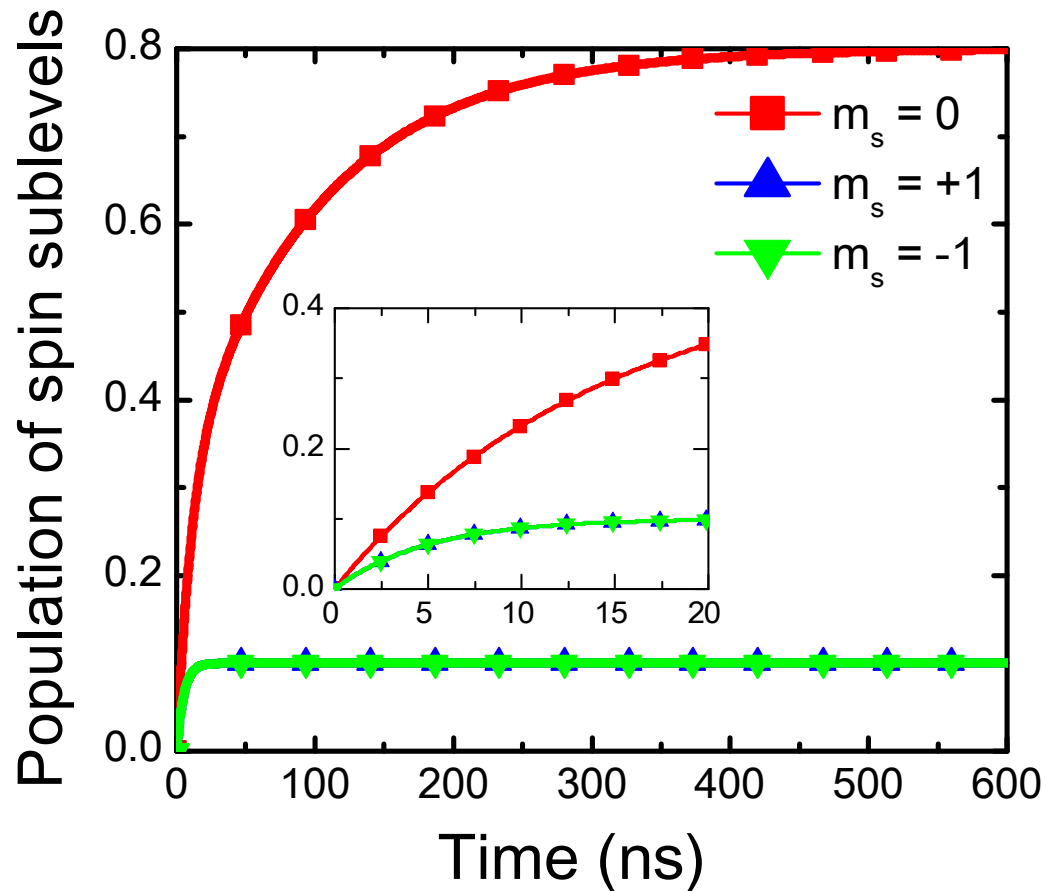
Phenomenological Master Equation:

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \sum_{i=1}^{16} k_i \left[P_i \rho P_i^\dagger - \frac{1}{2} (P_i^\dagger P_i \rho + \rho P_i^\dagger P_i) \right]$$

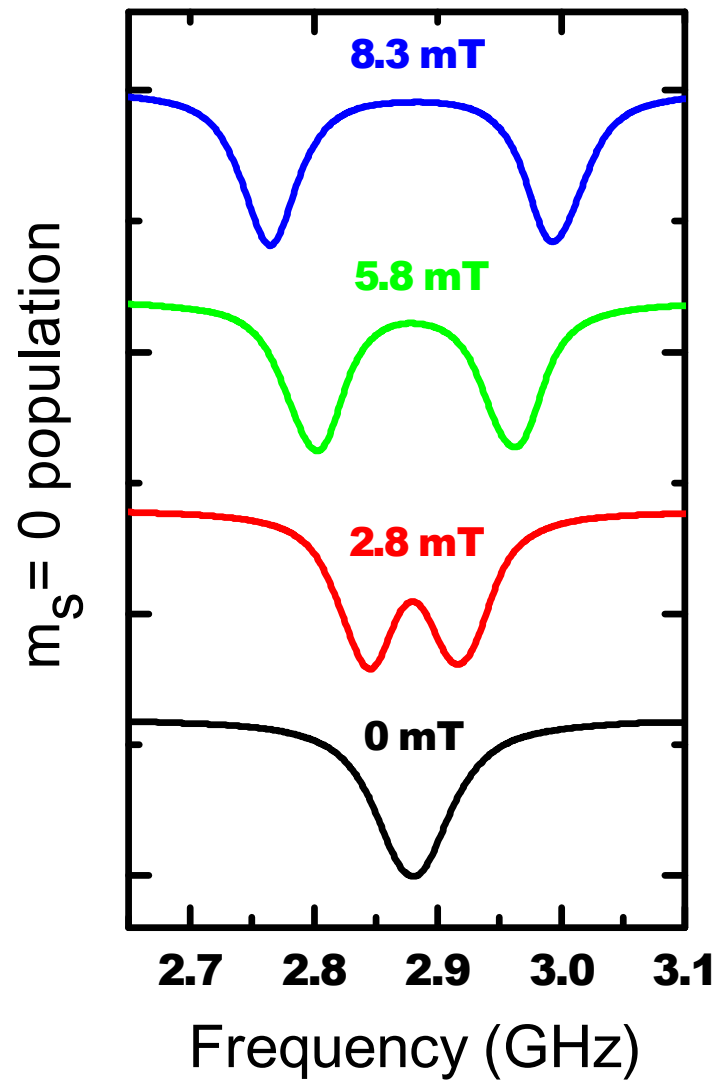
k_i is governed by various relaxation rates



Results



Optical Polarization



ODMR

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