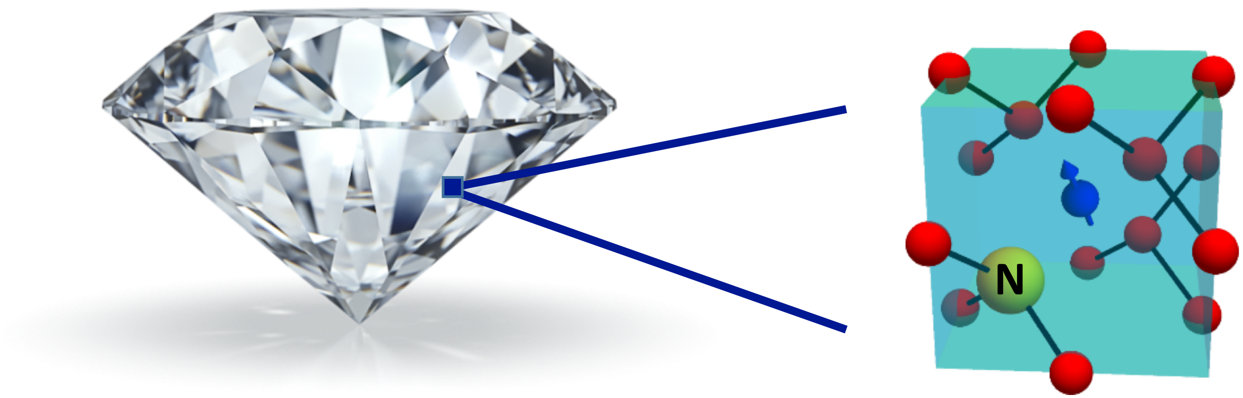
Quantum computing with the diamond NV centers

Hosung Seo

Physics Dept., Ajou University, Suwon, Republic of Korea

Diamond quantum computers



A quantum computer with this?

It seems .. yes! And it's even promising!

Toward a large-scale quantum computer

PRL **105**, 040504 (2010) PHYSICAL REVIEW LETTERS week ending 23 JULY 2010

Room-Temperature Implementation of the Deutsch-Jozsa Algorithm with a Single Electronic Spin in Diamond

Juliane Kniepert,[2]
Du[1,*]

LETTER Nature **484**, 82 (2012) doi:10.1038/nature10900

Decoherence-protected quantum gates for a hybrid solid-state spin register

T. van der Sar[1], Z. H. Wang[2], M. S. Blok[1], H. Ber
& V. V. Dobrovitski[2]

LETTER Nature **506**, 204 (2014). doi:10.1038/nature12919

Quantum error correction in a solid-state hybrid

ya[4], J. F. Du[5], P. Neumann[1]

A 10-qubit solid-state spin register with quantum memory up to one minute

C. E. Bradley[1,2,*] J. Randall[1,2,*] M. H. Abobeih[1,2], R. C. Berrevoets[1,2], M. J. Degen[1,2], M. A. Bakker[1,2], M. Markham[3], D. J. Twitchen[3], and T. H. Taminiau[1,2†]
[1] *QuTech, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands*
[2] *Kavli Institute of Nanoscience Delft, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands and*
[3] *Element Six, Fermi Avenue, Harwell Oxford, Didcot, Oxfordshire, OX11 0QR, United Kingdom*

arXiv:1905.02094
(Dated: May 7, 2019)

Grover's search algorithm using diamond

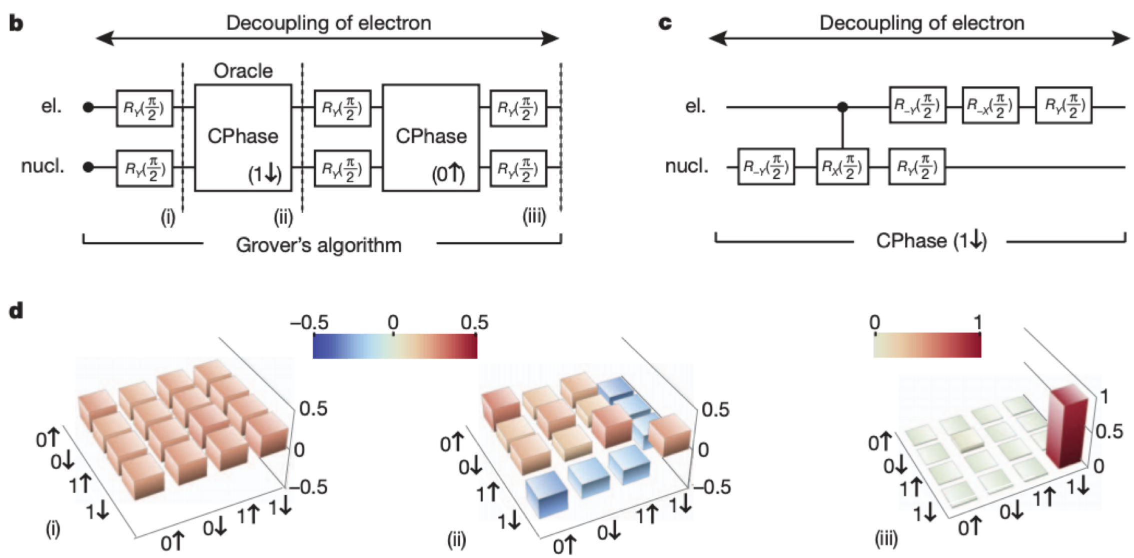
LETTER

Nature **484**, 82 (2012)

doi:10.1038/nature10900

Decoherence-protected quantum gates for a hybrid solid-state spin register

T. van der Sar[1], Z. H. Wang[2], M. S. Blok[1], H. Bernien[1], T. H. Taminiau[1], D. M. Toyli[3], D. A. Lidar[4], D. D. Awschalom[3], R. Hanson[1] & V. V. Dobrovitski[2]



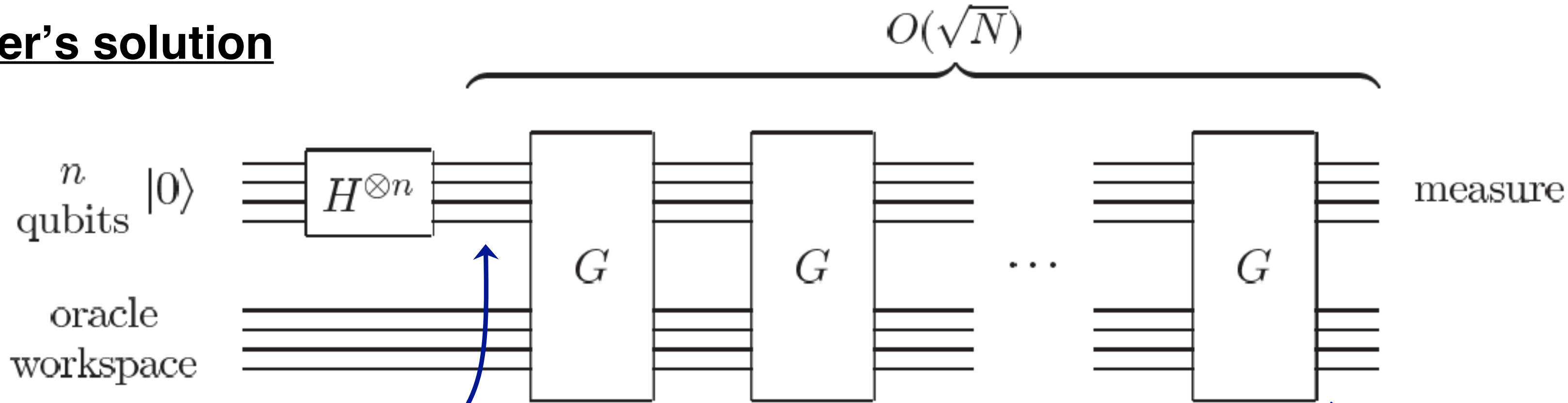
<u>Questions:</u> What are the basic ingredients to "realize" this?

<u>Goal:</u> Let's try to understand them one by one.

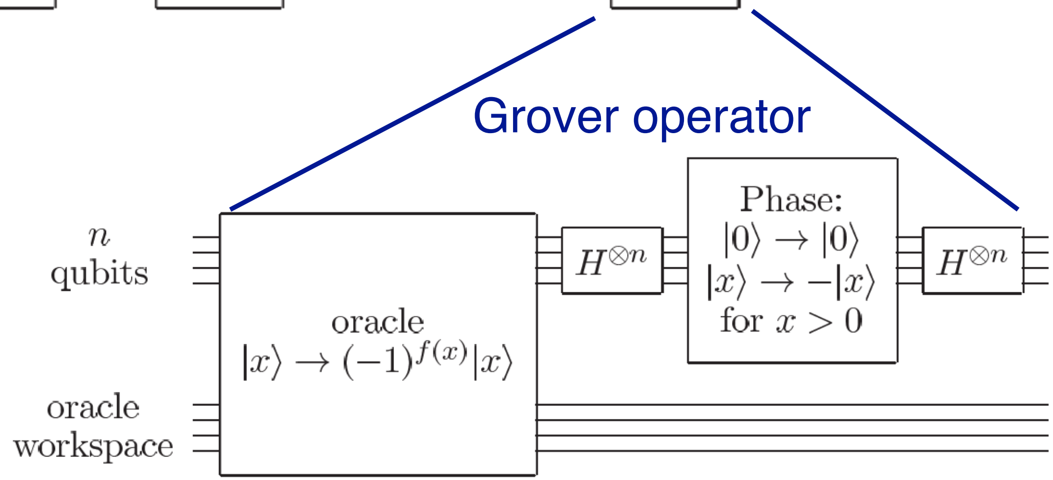
Grover's algorithm

Task: Find a solution to a search problem* in a search space of N elements using the smallest possible number of oracle** calls.

Grover's solution



$$|\psi\rangle = \frac{1}{N^{1/2}} \sum_{x=0}^{N-1} |x\rangle$$



***Search problem:**

$f(x) = 1$, if x is a solution

$f(x) = 0$, otherwise

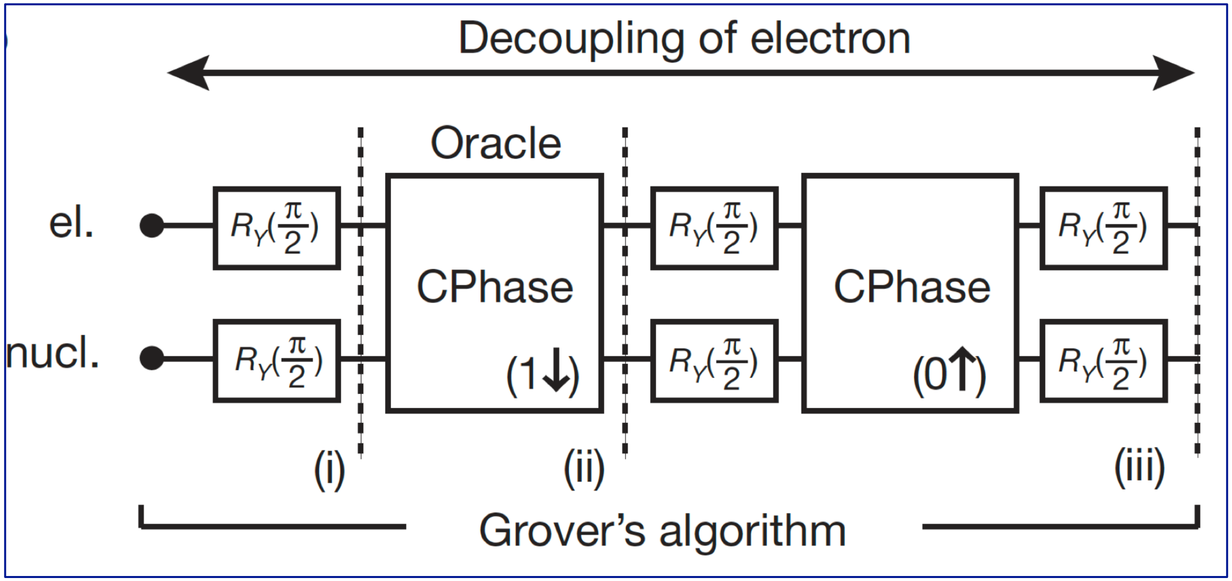
****Oracles can "recognize" solutions.**

Nielsen and Chuang (2000, Cambridge)

2-qubit Grover's algorithm

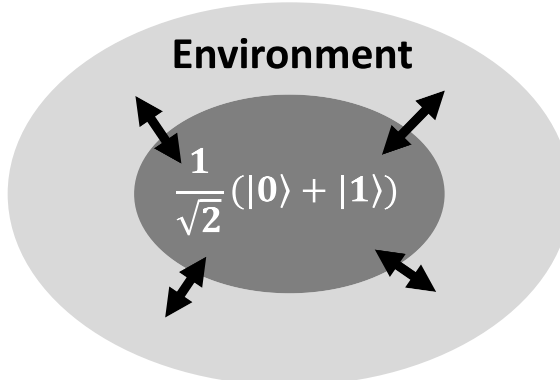
- There are only 4 elements in the database to search
  → 4 indices needed: $[0_e \uparrow_n]$, $[0_e \downarrow_n]$, $[1_e \uparrow_n]$, **$[1_e \downarrow_n]$** (solution)

- Only 1 Grover iteration is needed to rotate $|\psi\rangle$ to the target solution state.



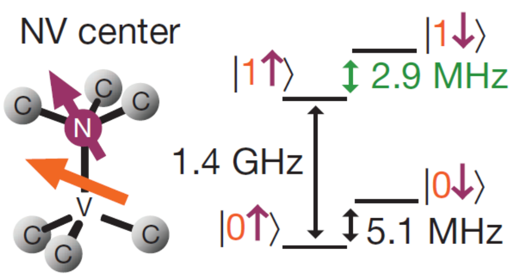
Van de Sar et al., Nature **484**, 82 (2012)

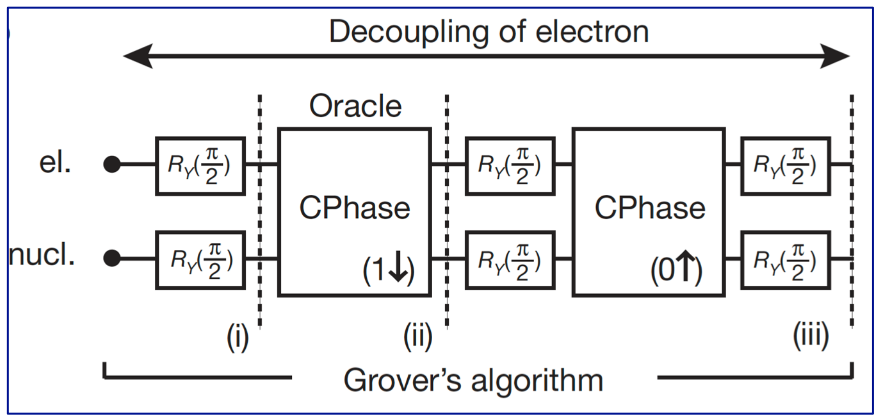
4 key components to understand & achieve

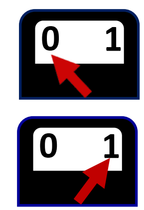


Decoherence and how to protect the register from it

2-qubit register & Initialization

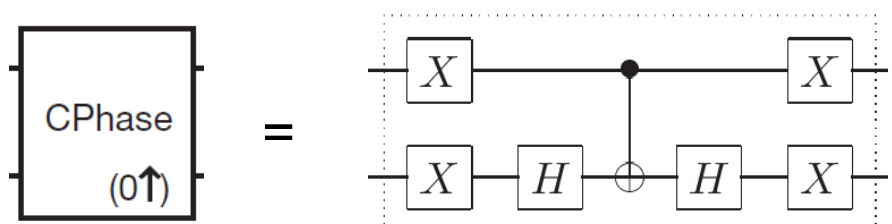






Readout

Single-qubit (Hadamard & X) and 2-qubit gates (CNOT)



Outline

1. **NV center as a solid-state qubit.**
   - Initialization and readout: Spin-dependent excitation and decay
   - Single-qubit operations via magnetic resonance

2. **NV – nuclear spin hybrid registers in diamond**
   - Nuclear spins in diamond (^{13}C and ^{14}N)
   - Spin Hamiltonian and 2-qubit gates

3. **Decoherence problem**
   - Qubits are open quantum systems
   - How to protect qubits from decoherence? Echo and dynamical decoupling

4. **Recent advances toward large-scale defect-based quantum computers**

Outline

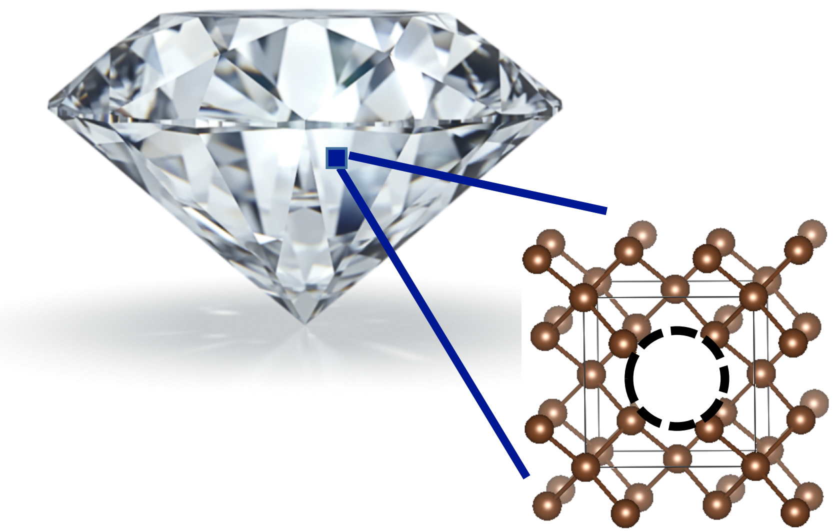
1. **NV center as a solid-state qubit.**
   - Initialization and readout: Spin-dependent excitation and decay
   - Single-qubit operations via magnetic resonance

2. **NV – nuclear spin hybrid registers in diamond**
   - Nuclear spins in diamond (^{13}C and ^{14}N)
   - Spin Hamiltonian and 2-qubit gates

3. **Decoherence problem**
   - Qubits are open quantum systems
   - How to protect qubits from decoherence? Echo and dynamical decoupling

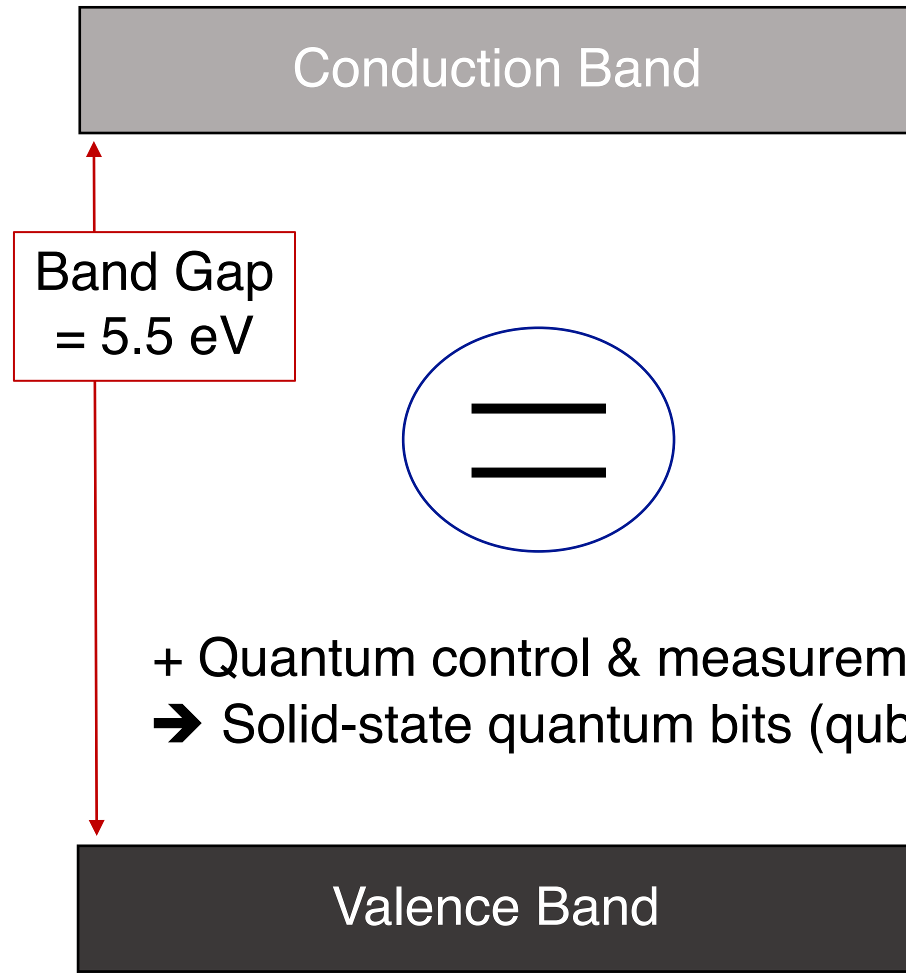
4. **Recent advances toward large-scale defect-based quantum computers**

Deep-level defects: Quantum states trapped in ‘crystal vacuum’



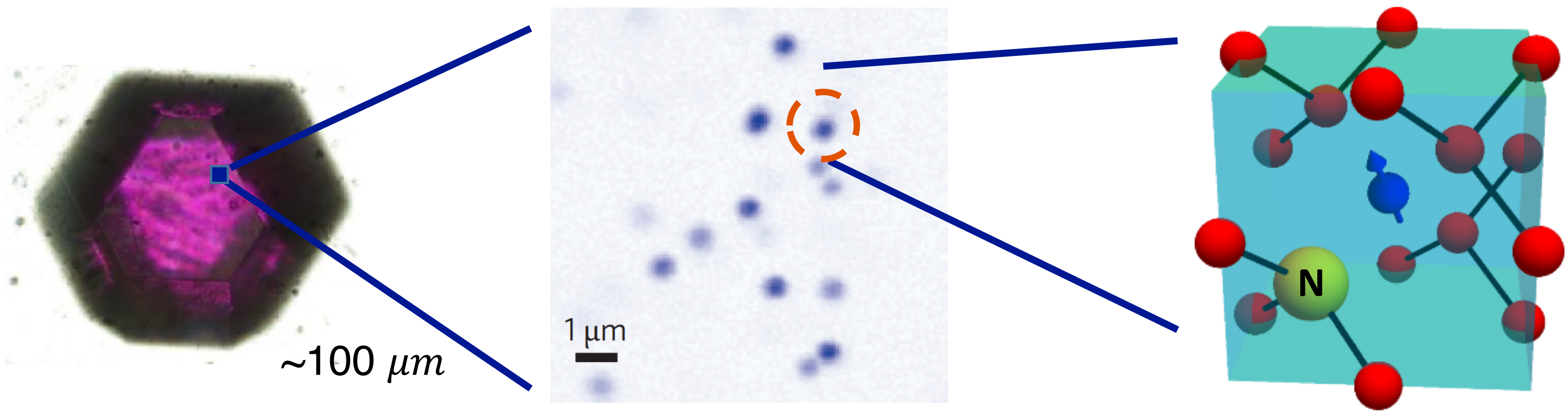
Color Centers

Boron | Nitrogen | Nitrogen-vacancy



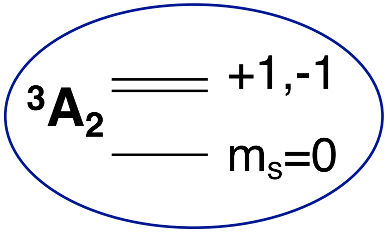
+ Quantum control & measurement
➔ Solid-state quantum bits (qubits)

Nitrogen-vacancy (NV) center in diamond



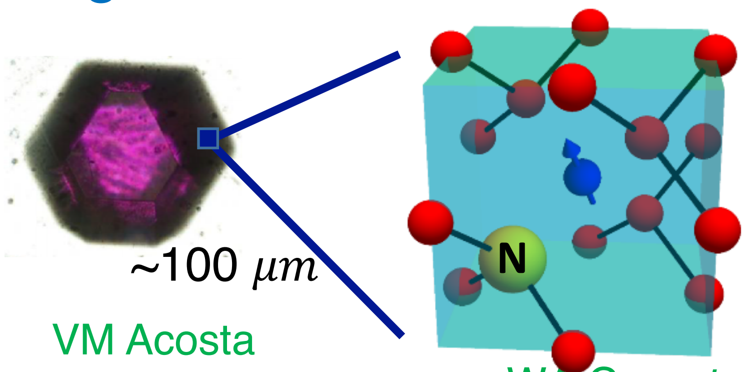
VM Acosta thesis (2011) WA Gao *et al.*, *Nat. Photon.* (2015).

- NV^- center = artificial 'ion' trapped in the solid-state
- Ground state with spin triplet (S=1)
- Long coherence time at 'room temperature'
- Single-spin optical addressability F Jelezko *et al. Phys. Rev. Lett. (*2004).



Initialization and readout of NV: Electronic structure matters.

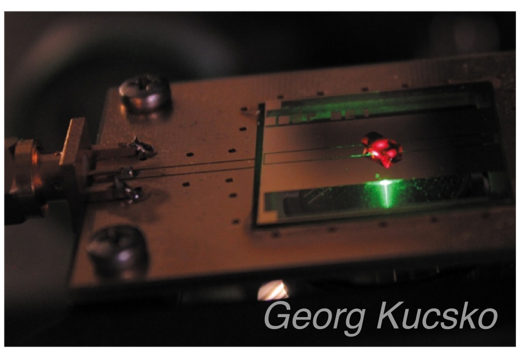
Singe NV centers

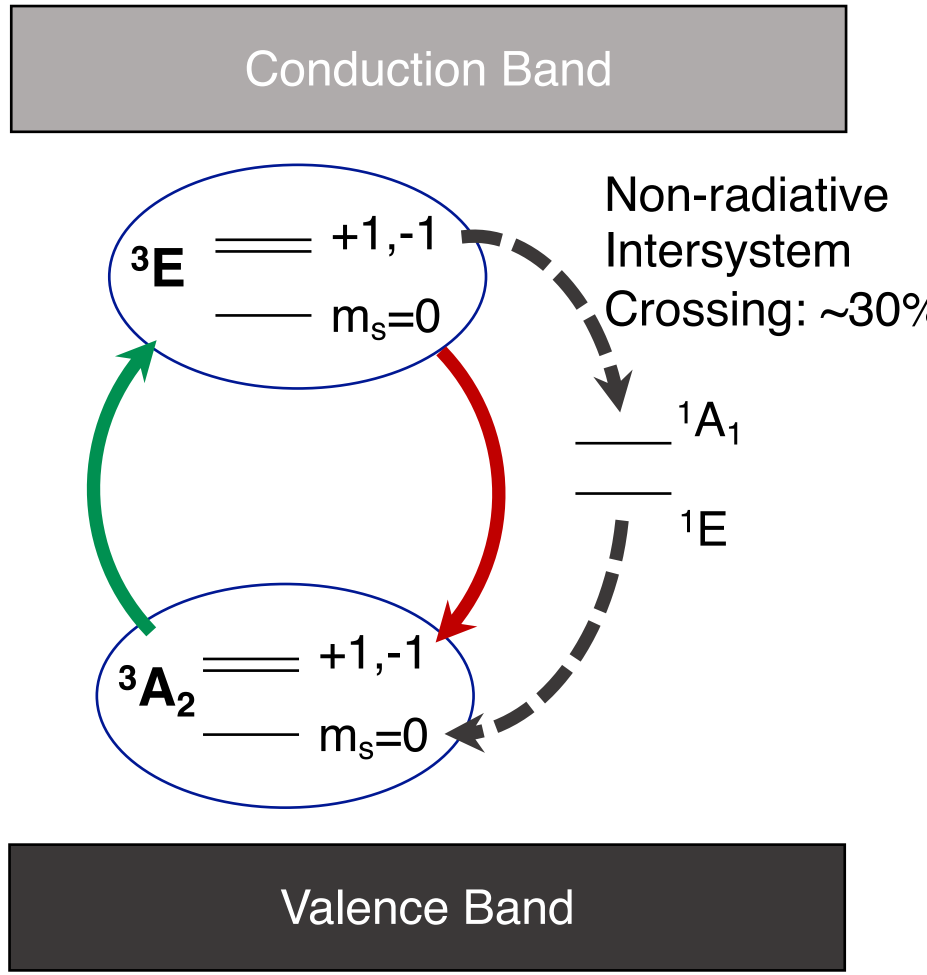


VM Acosta thesis (2011)

WA Gao *et al.* *Nat. Photon.* (2015).

Optical initialization and readout





F. Jelezko *et al.*, Phys. Rev. Lett. (2004).

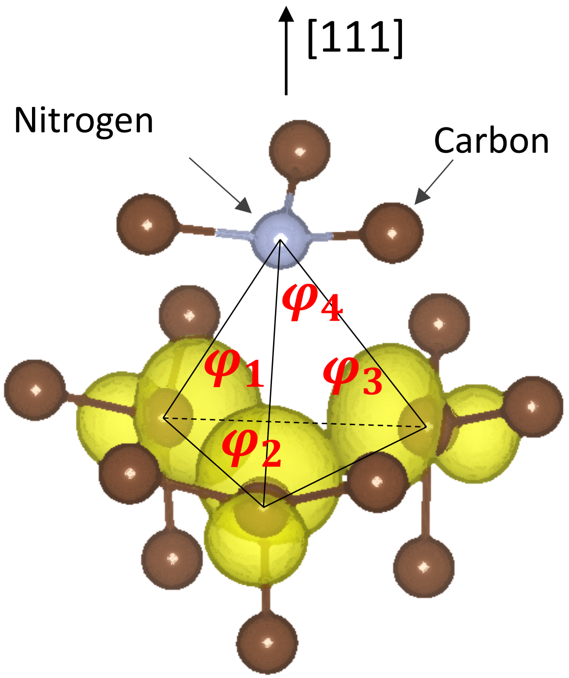
Electronic Structure of NV

Key aspects of the NV electronic structure

1. 6 electrons localized near the NV defect.
   - One from each C, two from N, and one from outside (i.e. a charged defects)

2. Single-electron basis functions
   - 3 C sp^3 dangling bonds ($\varphi_1, \varphi_2, \varphi_3$)
   - 1 N sp^3 dangling bondsform (φ_4)

3. Point group symmetry: C_{3v}



Character table of C_{3v}

	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

So, we need to solve a 6-electron problem with 4 orbitals in the C_{3v} symmetry embedded in a diamond. Then, how?

Electronic Structure of NV

Task flow

I. Find the symmetry-adopted wavefunctions.

II. Are they localized in the band gap? Then, find the ground state and excited state configurations.

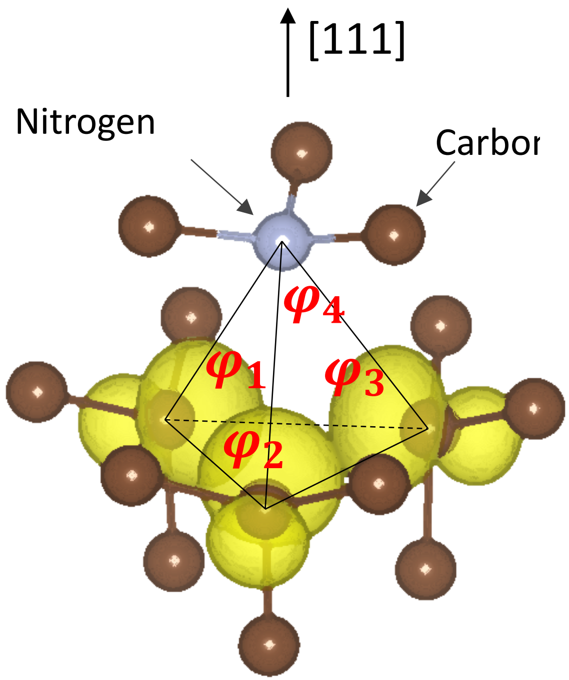
III. Consider the *e-e,* spin-spin & spin-orbit interactions. Construct many-electron states.

IV. Find out their energy ordering and the position with respect to the band edges

V. Dig into interesting physics: intersystem crossing, Lambda system, spin-photon, etc.

I. Symmetry-adopted basis functions of NV

C_{3v} point group symmetry



Character table for C_{3v}

	E	$2C_3$	$3\sigma_v$	Partners
A_1	1	1	1	z
A_2	1	1	-1	R_z
E	2	-1	0	x, y
Γ	4	1	2	$\varphi_{1,2,3,4}$

1) Find the matrix representation (Γ) using the 4 sp^3 hybrids as basis functions

$$O_R\varphi_j = \sum_i D_{ij}(R)\varphi_i \qquad \text{For } R = C_3^+ = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

[1] P.F. Bernath, *Spectra of atoms and molecules* (Oxford University Press, 1995)
[2] M.S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group theory* (Springer, 2008)

I. Symmetry-adopted basis functions of NV

2) Reduction of the representation:

$$\chi^{reducible}(C_k) = \sum_{\Gamma_j} a_j \chi^{\Gamma_j}(C_k)$$

$$\rightarrow a_j = \frac{1}{h}\sum_k N_k \chi^{\Gamma_j}(C_k)^* \chi^{reducible}(C_k)$$

a_{A1} = 2
a_{A2} = 0
a_E = 1

h = # of the group elements = 6 in our case
N_k = number of elements in the class C_k

$\Gamma = 2A_1 \oplus 1E$

3) Projection operator $P^{\Gamma_n} = \left(\frac{l_n}{h}\right)\sum_R \chi^{\Gamma_n}(R) O_R$ l_n = dimensionality of Γ_n

$$P^{A_1} = (\mathrm{E} + C_3^+ + C_3^- + \sigma_1 + \sigma_2 + \sigma_3)/6$$
$$P^{A_2} = (\mathrm{E} + C_3^+ + C_3^- - \sigma_1 - \sigma_2 - \sigma_3)/6$$
$$P^E = 2(2\mathrm{E} - C_3^+ - C_3^-)/6$$

[1] P.F. Bernath, *Spectra of atoms and molecules* (Oxford University Press, 1995)
[2] M.S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group theory* (Springer, 2008)

I. Symmetry-adopted basis functions of NV

3) Apply the projection operator to each sp³ hybrid to obtain the symmetry-adopted basis functions

$$P^{A_1}\varphi_i(i=1,2,3)=\frac{1}{3}(\varphi_1+\varphi_2+\varphi_3)$$

$$P^{A_1}\varphi_4=\varphi_4$$

$$P^{E}\varphi_1=\frac{2}{6}(2\varphi_1-\varphi_2-\varphi_3)$$

Also do $P^{E}\varphi_2$ & $P^{E}\varphi_3$

4) Normalization and extra mixing allowed by symmetry.

Gram-Schmidt

$$a_1(N)=\varphi_4$$
$$a_1(C)=(\varphi_1+\varphi_2+\varphi_3)/\sqrt{3}$$
$$e_x=(2\varphi_1-\varphi_2-\varphi_3)/\sqrt{6}$$
$$e_y=(\varphi_2-\varphi_3)/\sqrt{2}$$

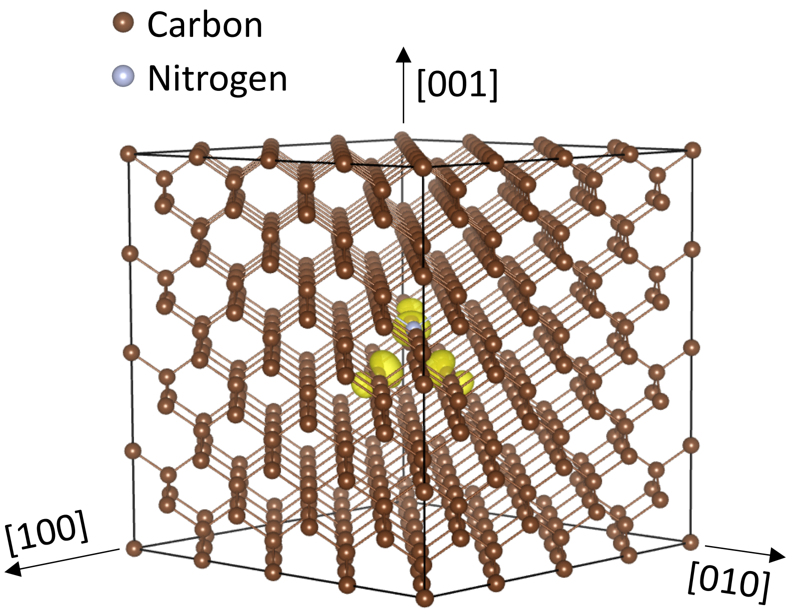
Consider mixing →

$$a_1(1)=\sqrt{1-\alpha^2}\varphi_4-\frac{\alpha}{\sqrt{3}}\sum_i^3\varphi_i$$
$$a_1(2)=\alpha\varphi_4+\sqrt{\frac{1-\alpha^2}{3}}\sum_i^3\varphi_i$$
$$e_x=(2\varphi_1-\varphi_2-\varphi_3)/\sqrt{6}$$
$$e_y=(\varphi_2-\varphi_3)/\sqrt{2}$$

II. Ground- and excited-state configuration

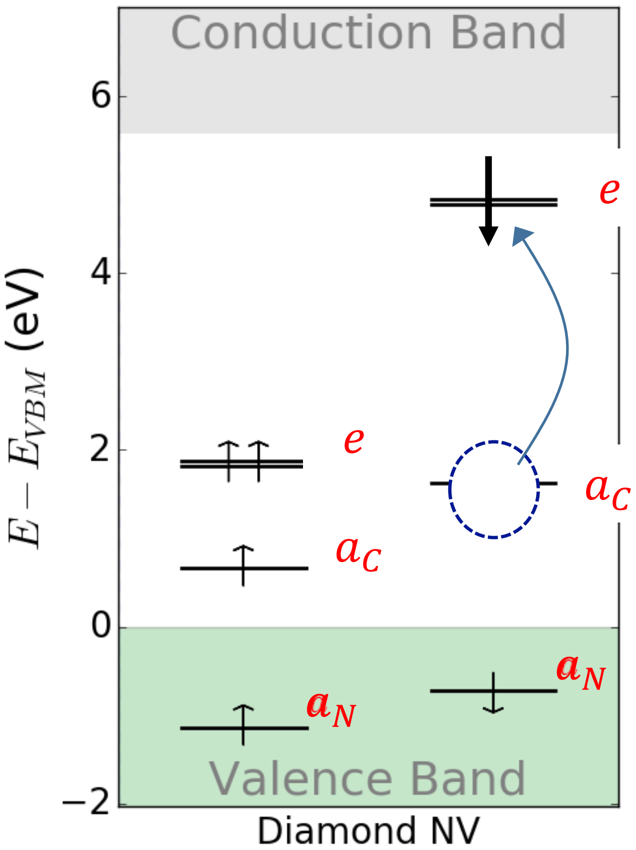
MOs' energy with respect to the band edge

1. Tight-binding calculations
2. Density functional theory (Hybrid or GW)



Ground-state:	$a_N^2\ a_c^2\ e^2$
1st excited-state:	$a_N^2\ a_c^1\ e^3$

Defect-level diagram

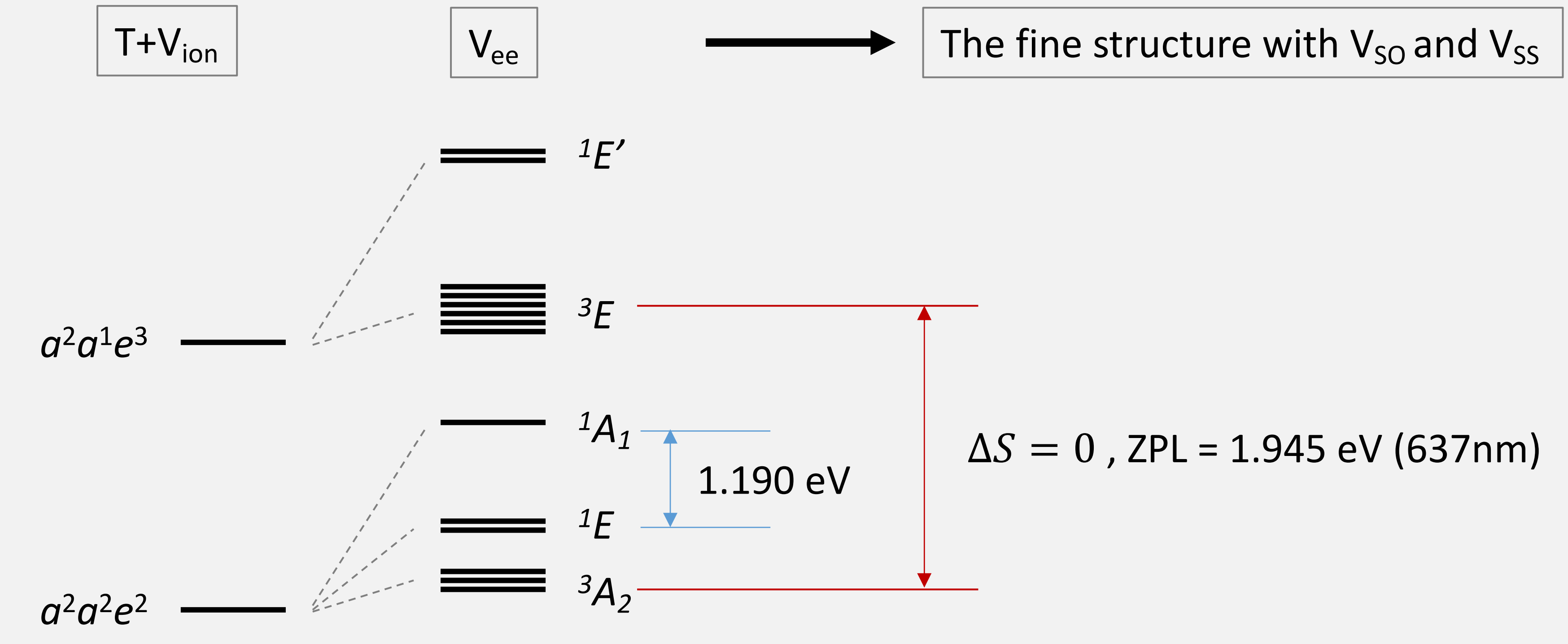


e-*e*, spin-spin, and spin-orbit interactions

e-e interaction: Hubbard model + Exact Diagonalization + Sym. analysis

$$H = \sum_{i\sigma} E_i n_{i\sigma} + \sum_{i \neq j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} U n_i n_j + \sum_{i>j,\sigma\sigma'} V n_{i\sigma} n_{j\sigma'}$$

Choi, Jain, and Louie, PRB (2012).

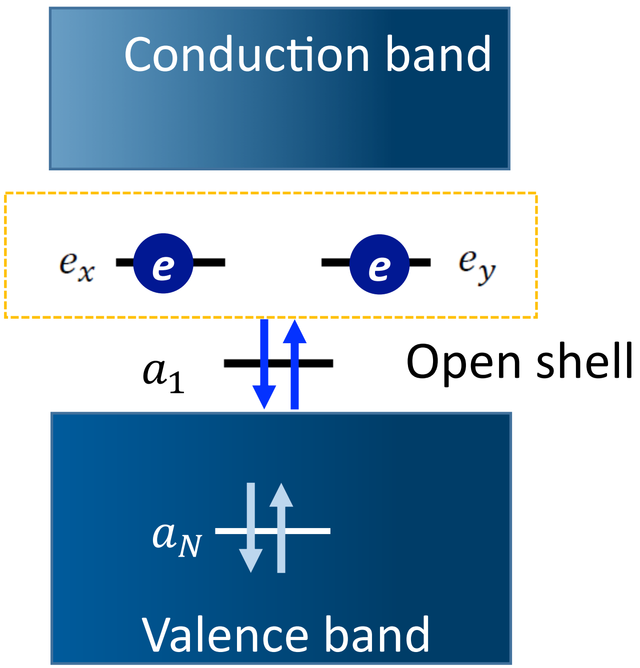


Doherty, Manson, Delaney, and Hollenberg, New J. Phys. **13**, 025019 (2011).

e-e & spin-spin: A simpler way

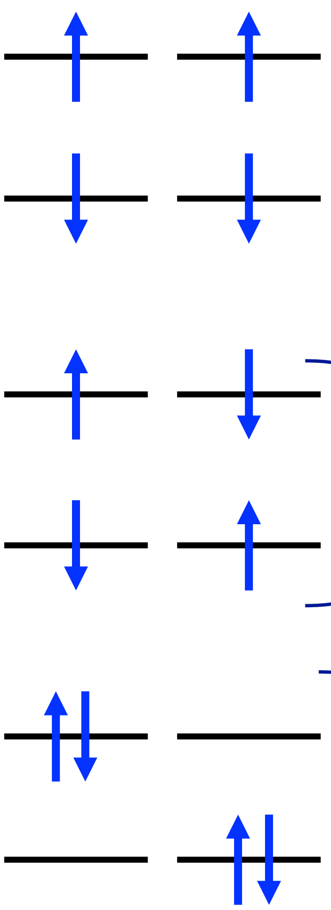
Ground-state configuration

$a^2 a^2 \mathbf{e^2}$



$$E \otimes E = A_1 \oplus A_2 \oplus E$$

Possible spin configurations



$$|e_x e_y - e_y e_x\rangle \otimes |\uparrow\uparrow\rangle$$

$$|e_x e_y - e_y e_x\rangle \otimes |\downarrow\downarrow\rangle$$

$$|e_x e_y - e_y e_x\rangle \otimes |\uparrow\downarrow + \downarrow\uparrow\rangle$$

$\}\ ^3A_2$

$$|e_x e_y + e_y e_x\rangle \otimes |\uparrow\downarrow - \downarrow\uparrow\rangle$$

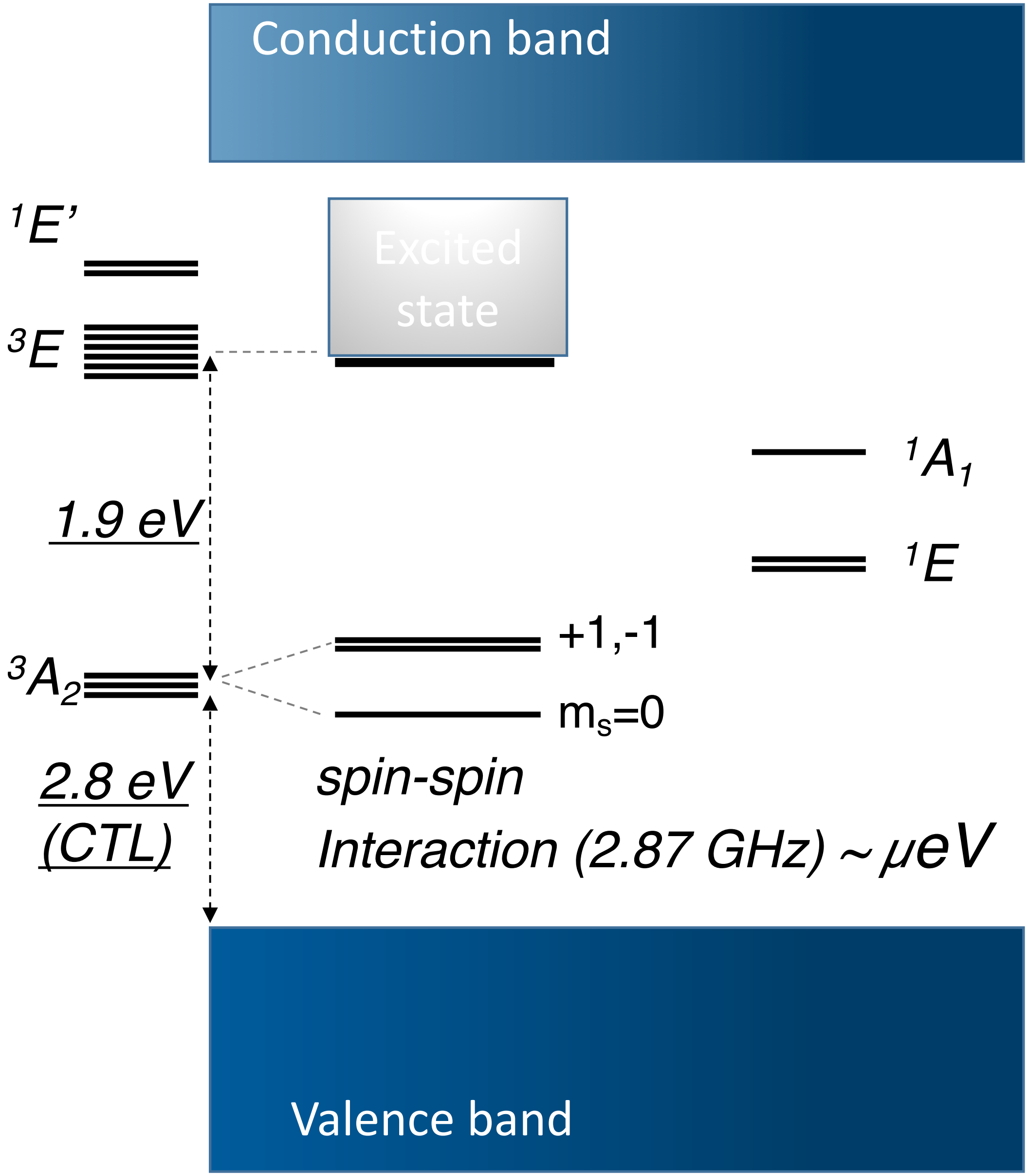
$$|e_x e_x - e_y e_y\rangle \otimes |\uparrow\downarrow - \downarrow\uparrow\rangle$$

$\}\ ^1E$

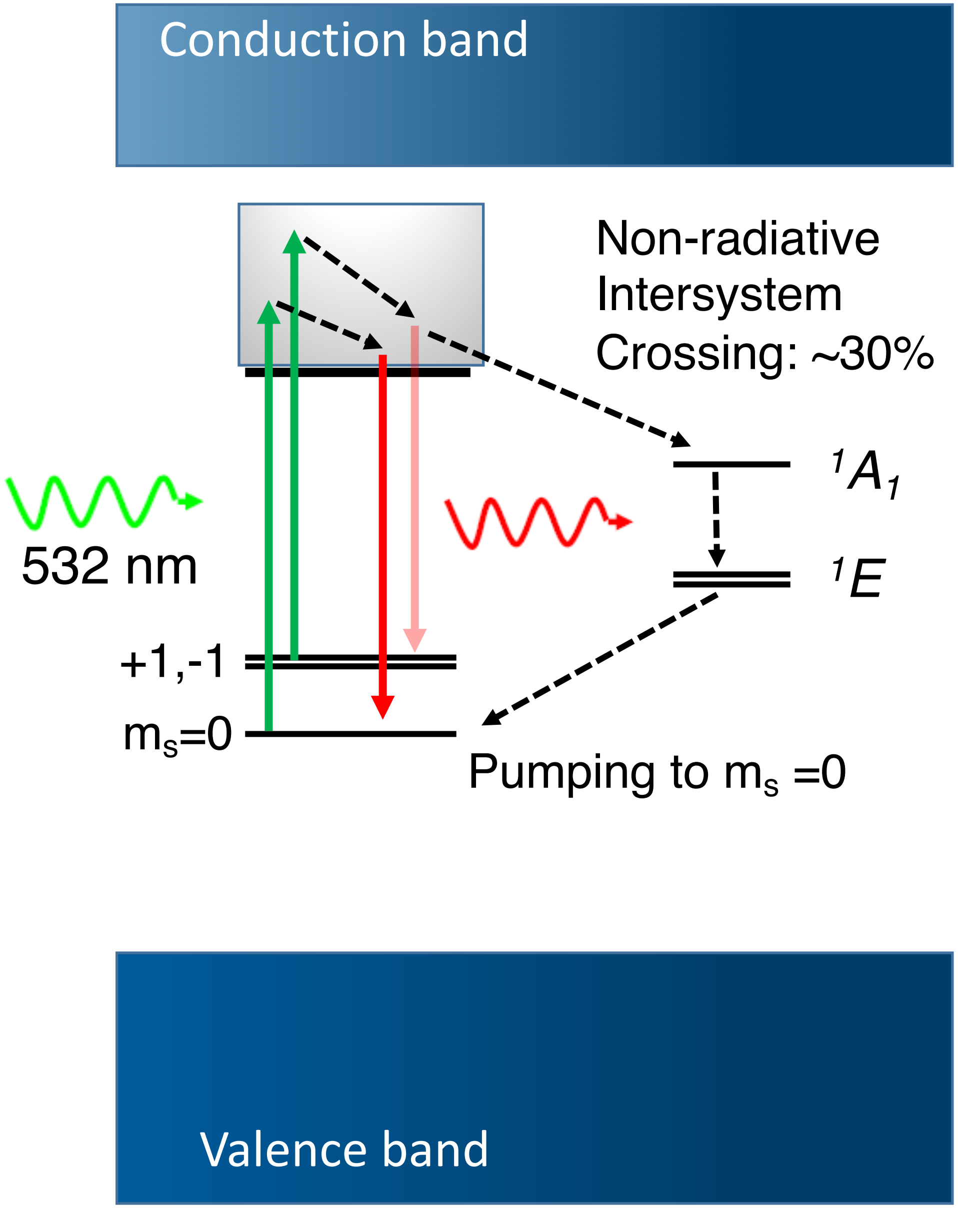
$$|e_x e_x + e_y e_y\rangle \otimes |\uparrow\downarrow - \downarrow\uparrow\rangle$$

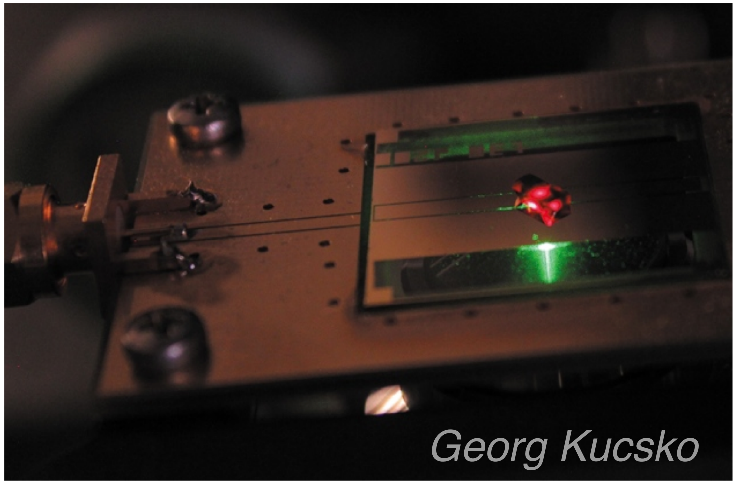
$\}\ ^1A_1$

Optical Initialization and Readout

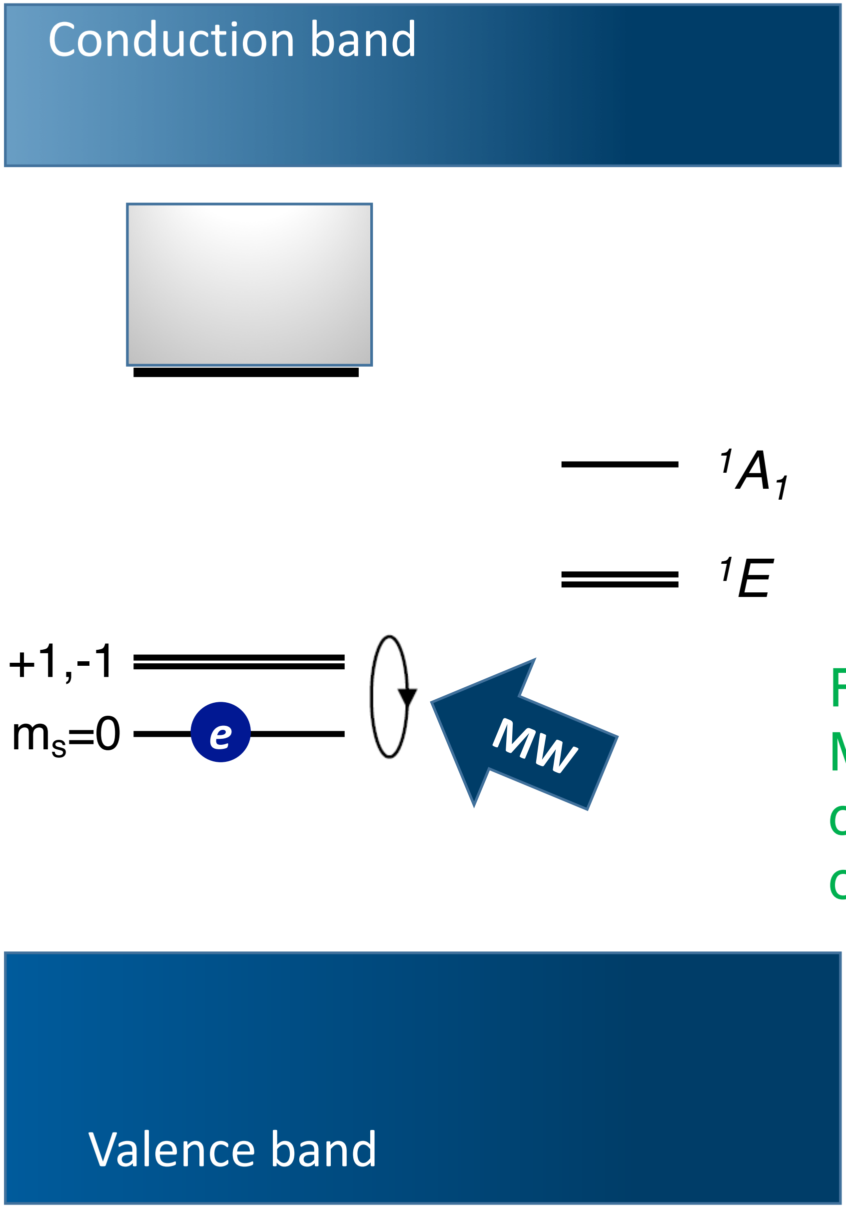


Optical pumping to m_s = 0: Initialization



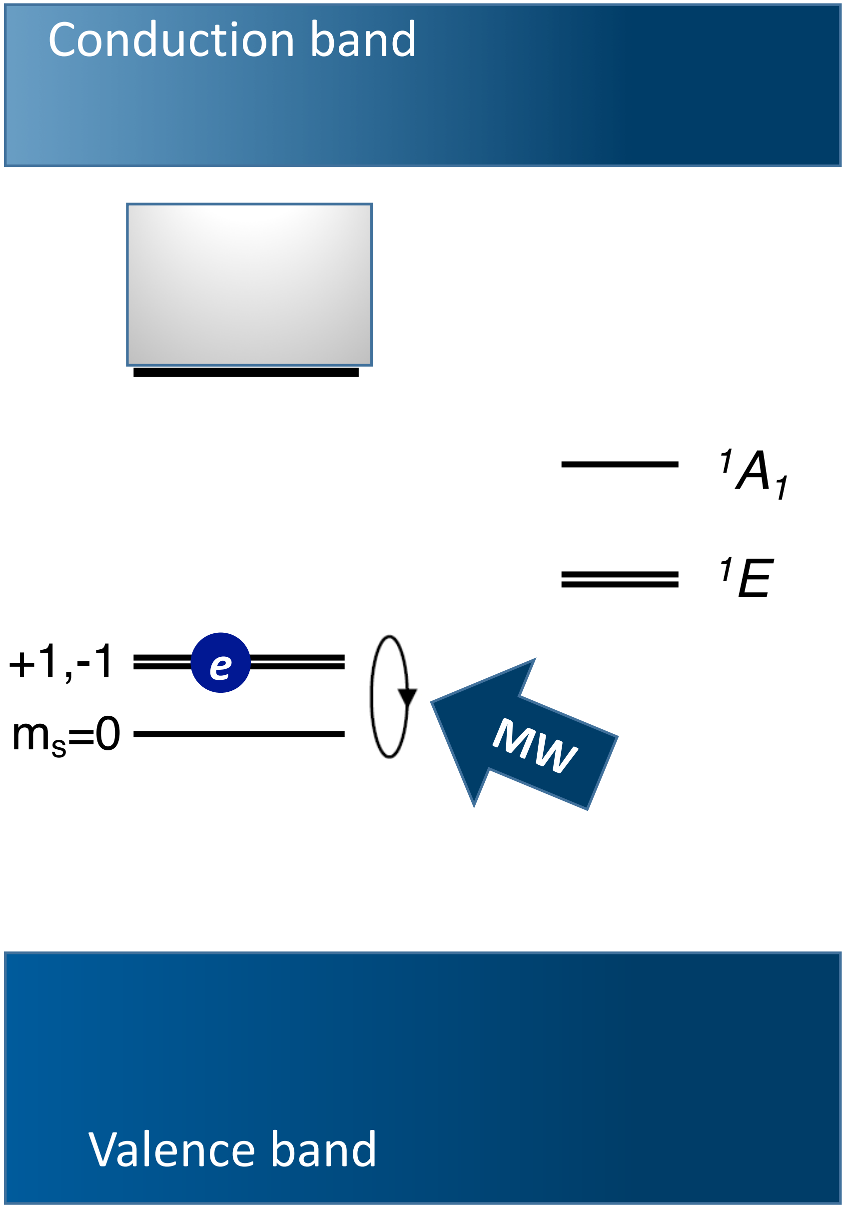


Microwave driving of NV spin state

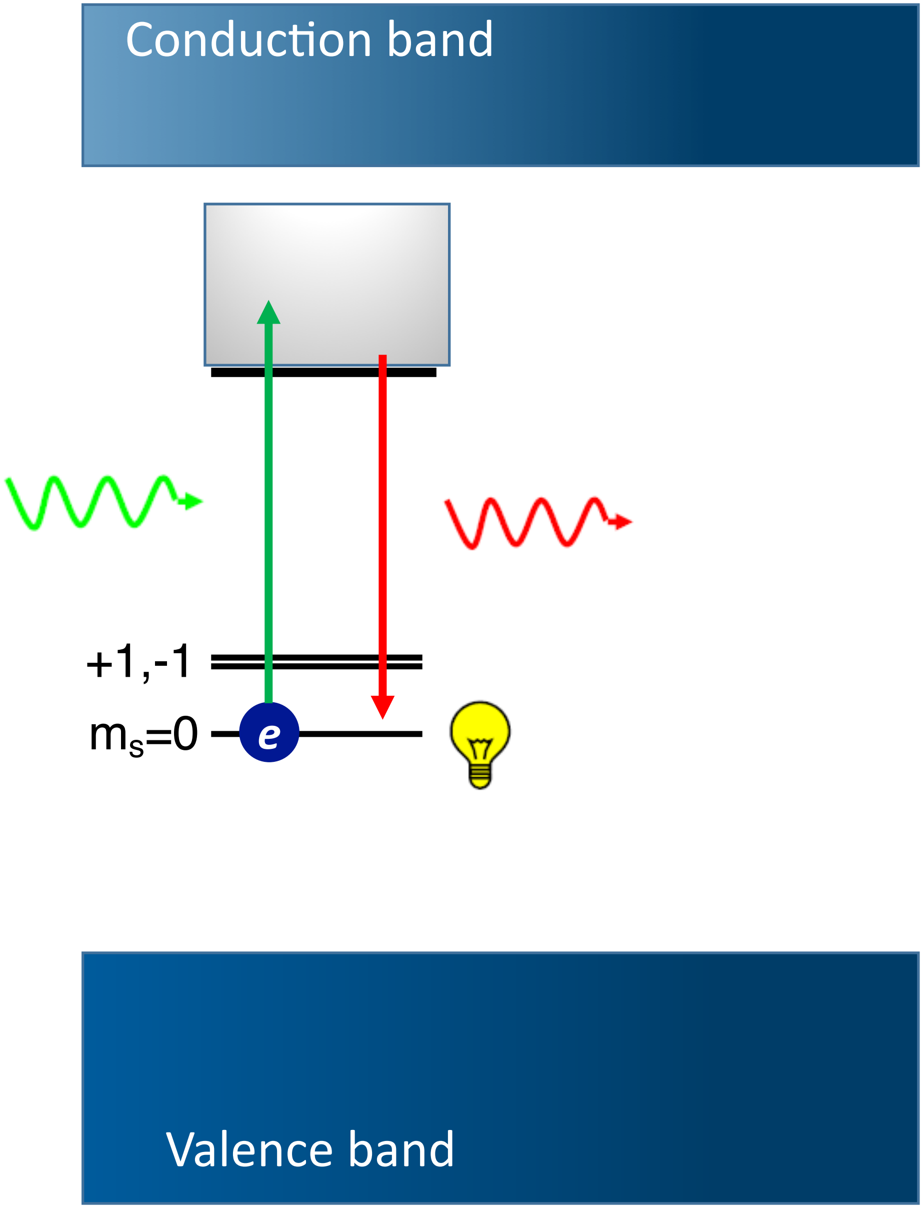


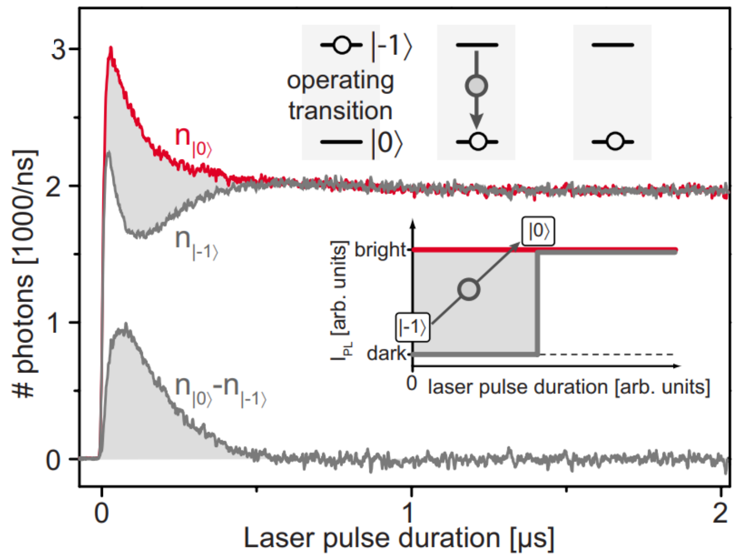
For the detailed description of the MW-driven magnetic resonance control, see, e.g., the lecture note of Prof. Dohun Kim.

Microwave driving of NV spin state



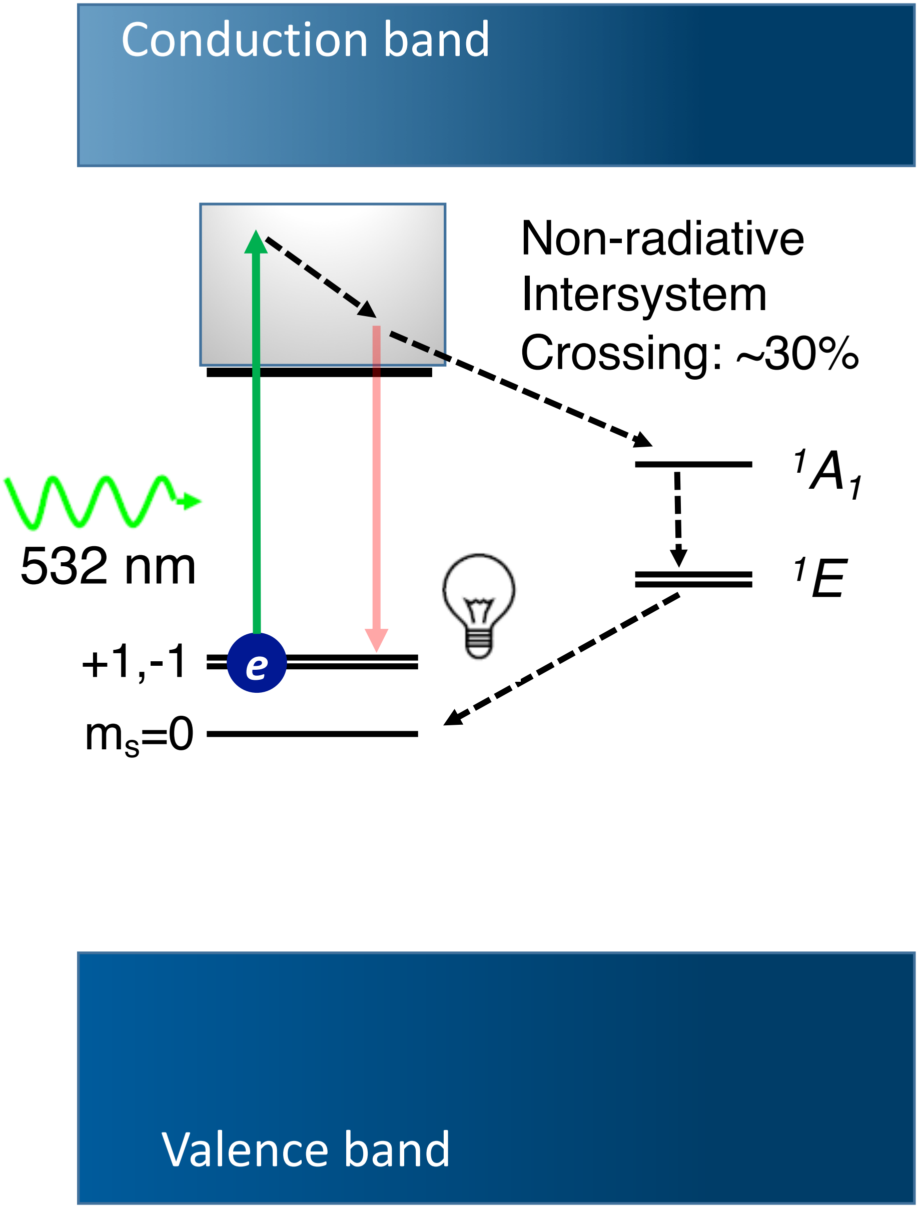
Optical spin-state readout: m_s=0 bright state

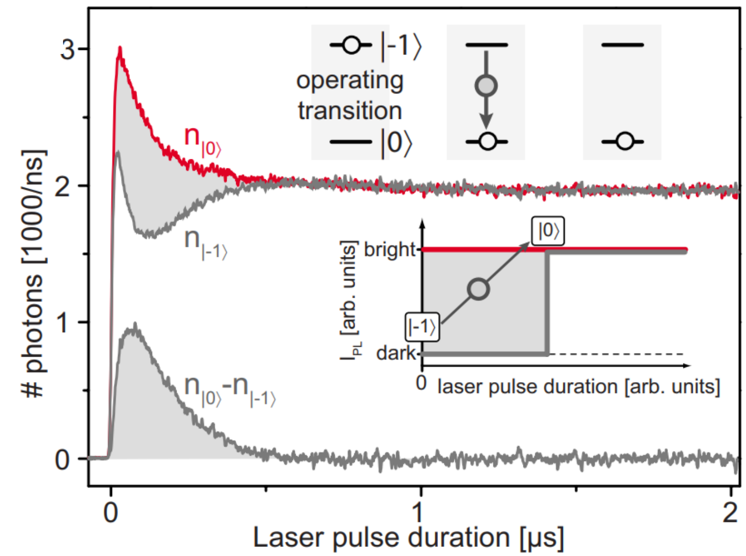




M. Steiner et al., PRB (2010).

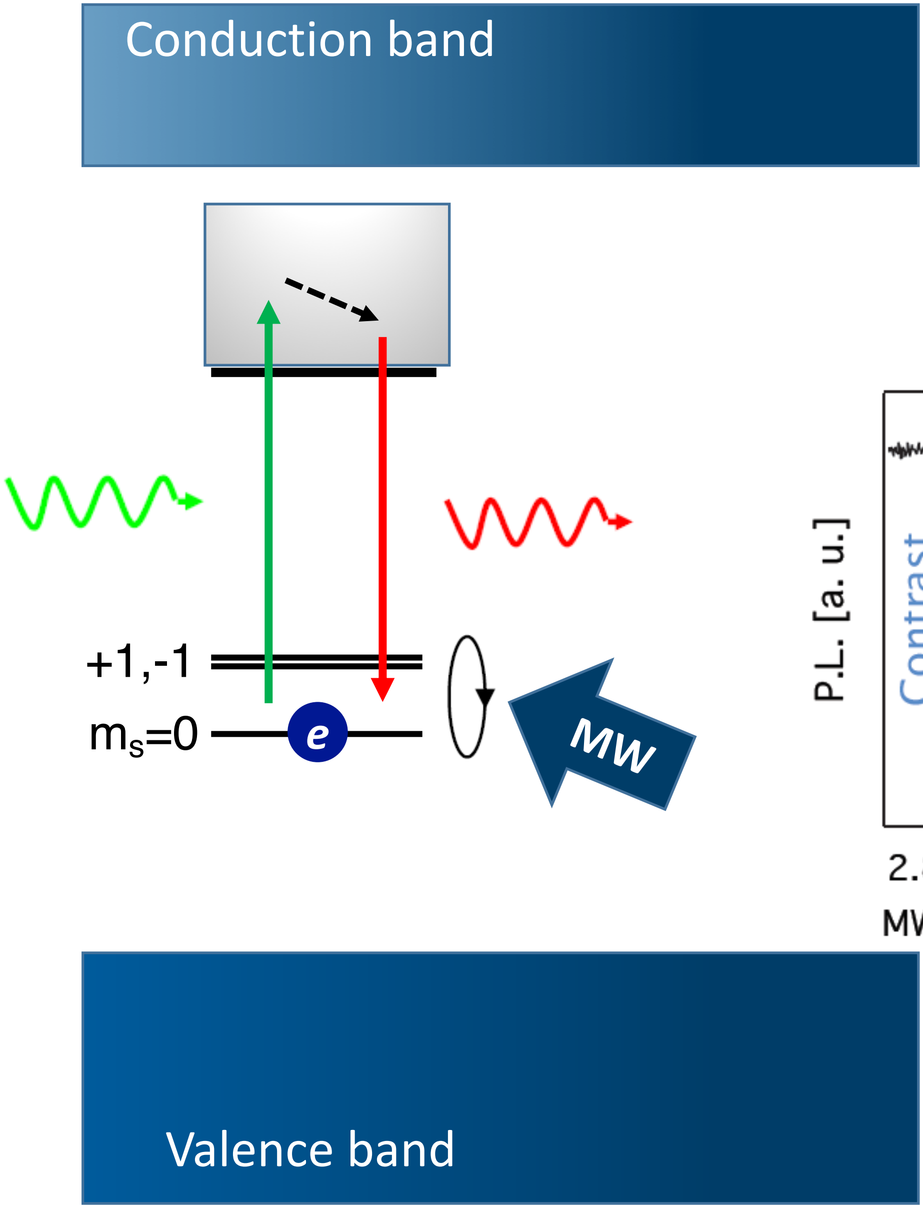
Optical spin-state readout: dark states

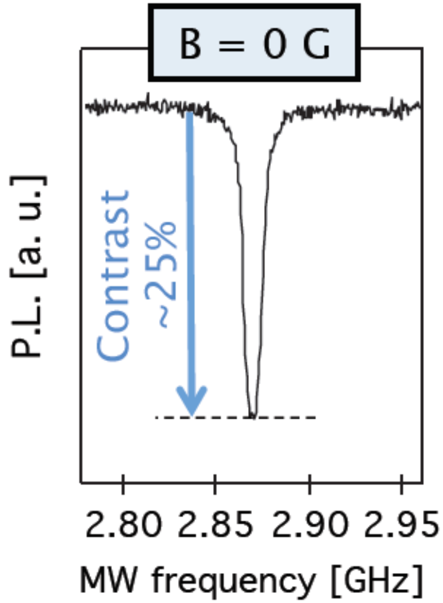




M. Steiner et al., PRB (2010).

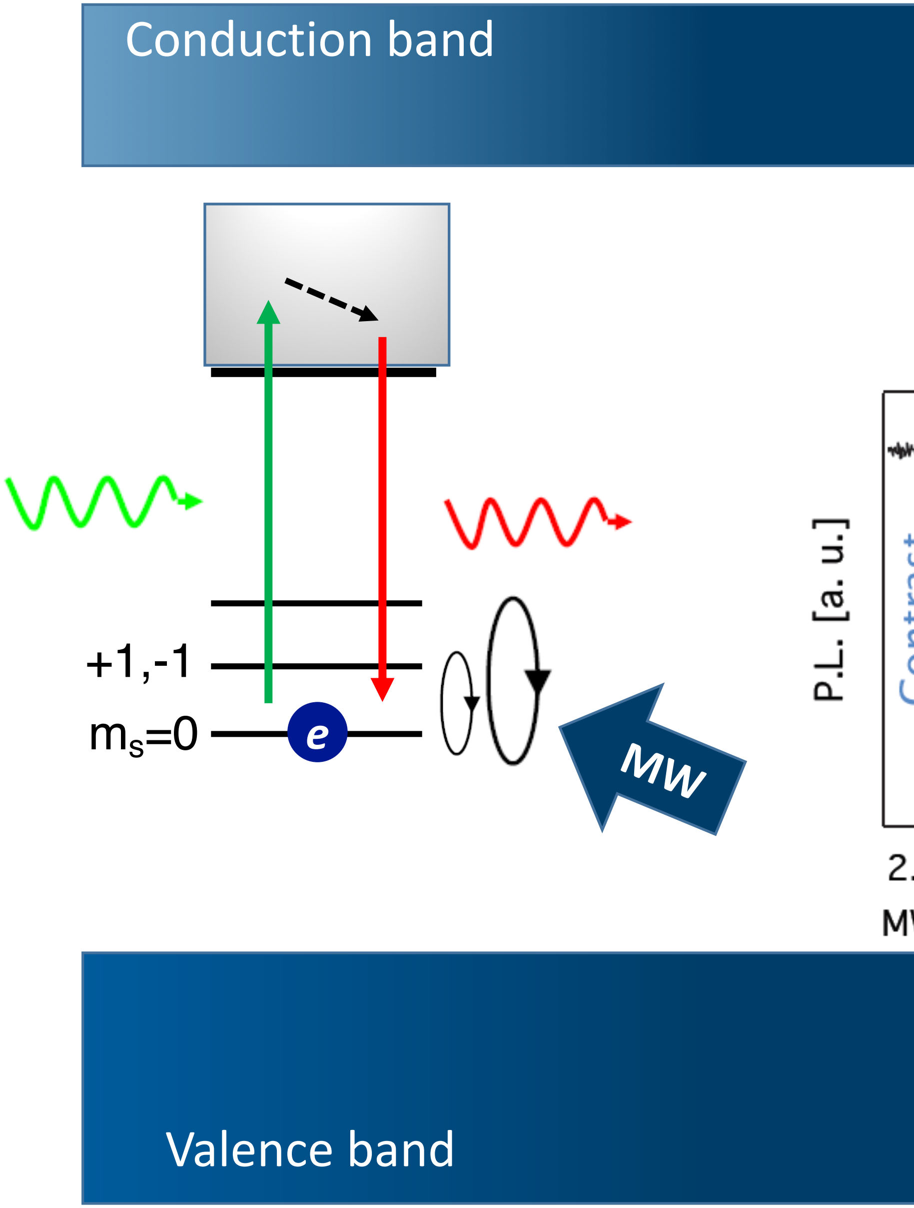
Optically detected magnetic resonance

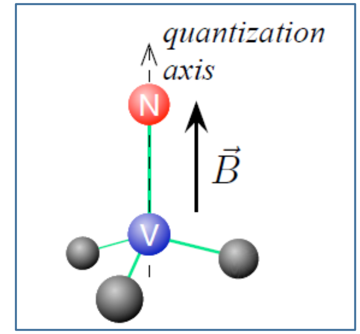


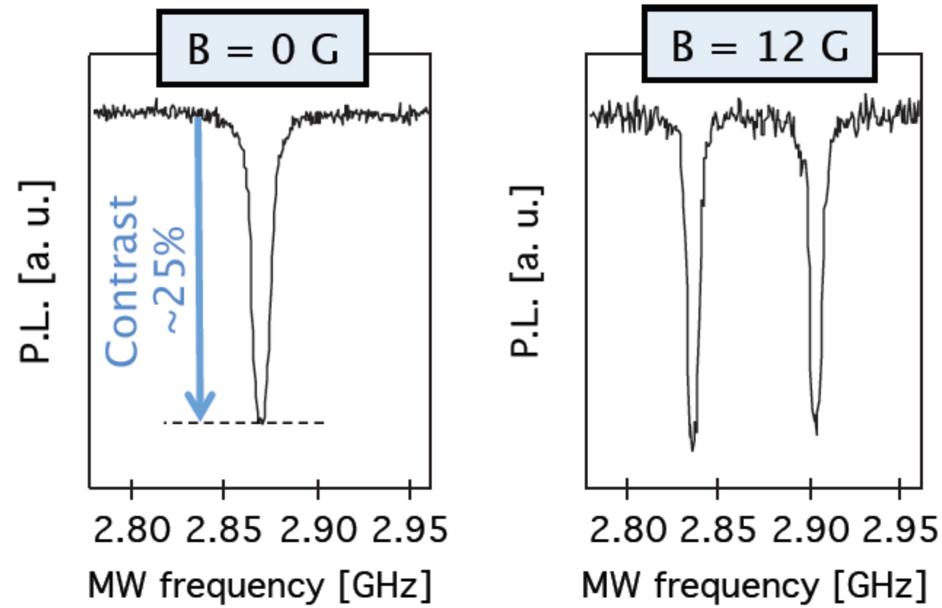


A. Dreau *et al.*, GDR IQFA 2nd workshop (2012).

Optically detected magnetic resonance



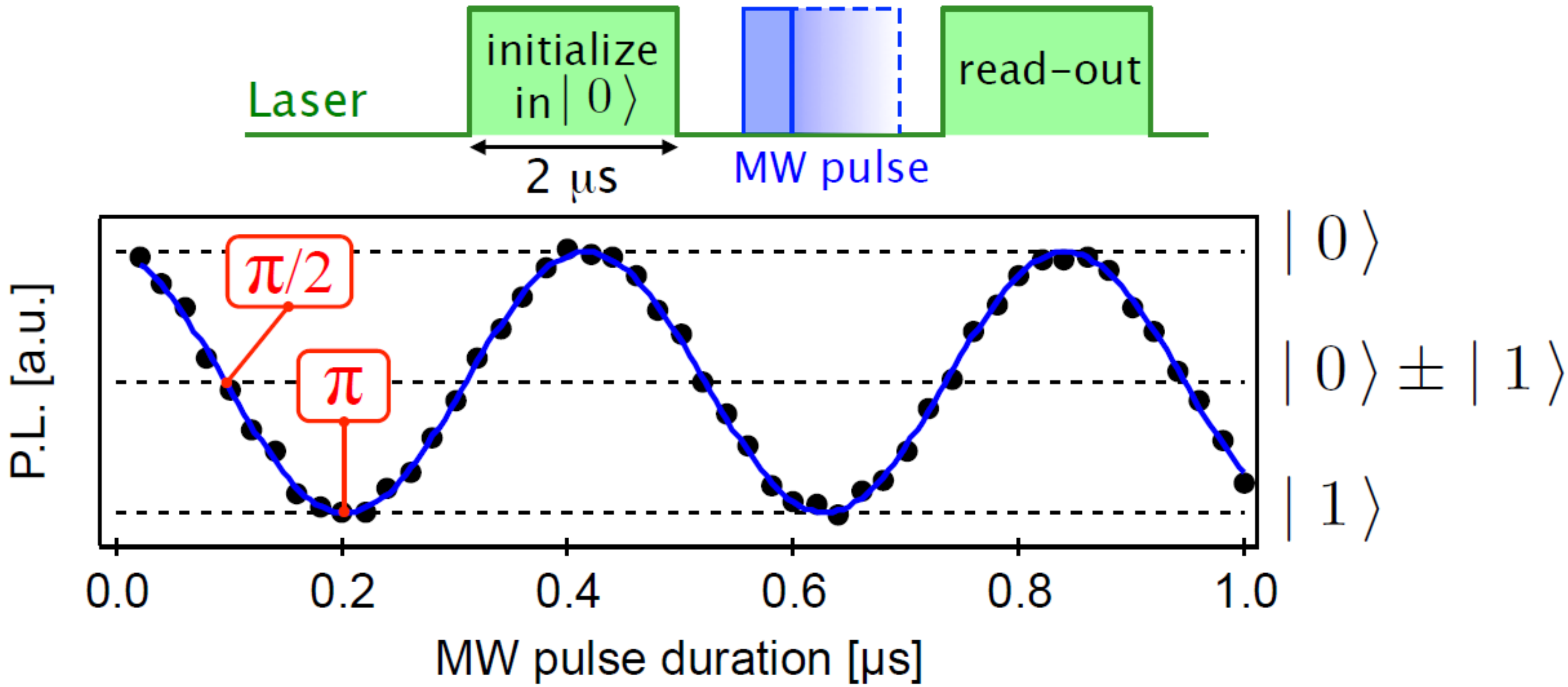




A. Dreau *et al.*, GDR IQFA 2nd workshop (2012).

NV as a single qubit device

- Rabi oscillation



A. Dreau *et al.*, GDR IQFA 2nd workshop (2012).

Outline

1. **NV center as a solid-state qubit.**
   - Initialization and readout: Spin-dependent excitation and decay
   - Single-qubit operations via magnetic resonance

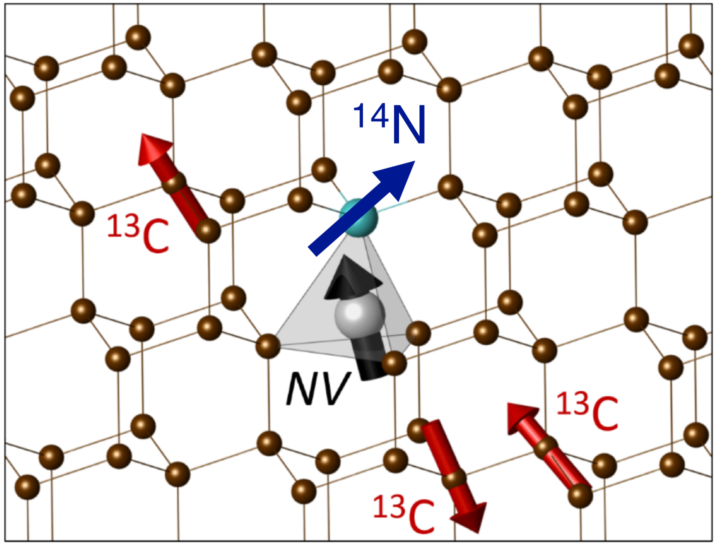
2. **NV – nuclear spin hybrid registers in diamond**
   - Nuclear spins in diamond (^{13}C and ^{14}N)
   - Spin Hamiltonian and 2-qubit gates

3. **Decoherence problem**
   - Qubits are open quantum systems
   - How to protect qubits from decoherence? Echo and dynamical decoupling

4. **Recent advances toward large-scale defect-based quantum computers**

Hybrid spin registers in diamond

Nuclear spin environment in diamond



Carbon isotopes

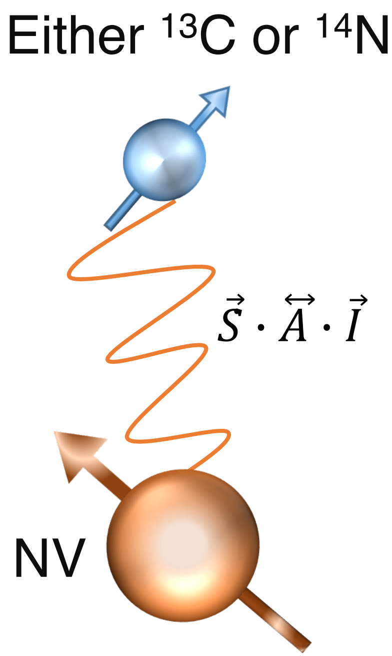
	Mass	Natural abund.	Nuclear spin (I)	Magnetic moment (μ/μ_N)
^{12}C	12.000	98.93 %	0	0
^{13}C	**13.003**	**1.07 %**	**1/2**	**0.702**

N isotopes

	Mass	Natural abund.	Nuclear spin (I)	Magnetic moment (μ/μ_N)
^{14}N	**14.003**	**99.63 %**	**1**	**0.404**
^{15}N	15.000	0.368 %	1/2	-0.283

http://www.webelements.com/

Hybrid spin registers in diamond



Nuclear spins in diamond as qubits

- Advantages: Long T_2 (coherence) and T_1 (relaxation) due to very small spin-environment coupling (γ_n).
- Disadvantage: Ironically, small γ_n means little controllability: they are hard to detect and manipulate at the single-spin levels.

NV electronic spins in diamond as qubits

- Advantages: Optical initialization and readout at the single-spin level. Fast MW control due to its large γ_e. Can couple with various degrees of freedom in solids (spin, photon, phonon, strain, etc.)
- Disadvantage: Relatively short memory time.

➔ Use NV and nuclear spins as a hybrid register

- NV and nearby nuclear spins can be coherently coupled via hyperfine interaction.
- NV can be used as an ancillary qubit to control and detect the nuclear spins.

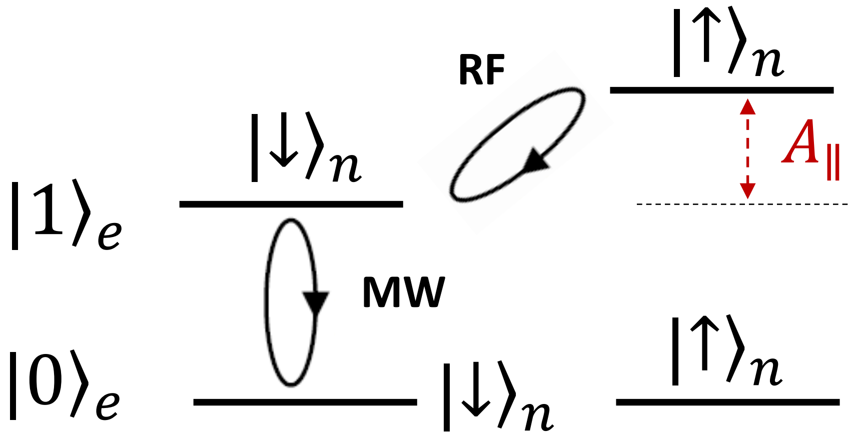
M. V. Dutt et al., Science **316**, 1312 (2007).
P. Neumann et al., Science **320**, 1326 (2008).
T. Van der Sar et al., Nature **484**, 82 (2012).
C. E. Bradley et al., arXiv 1905:02094 (2019).

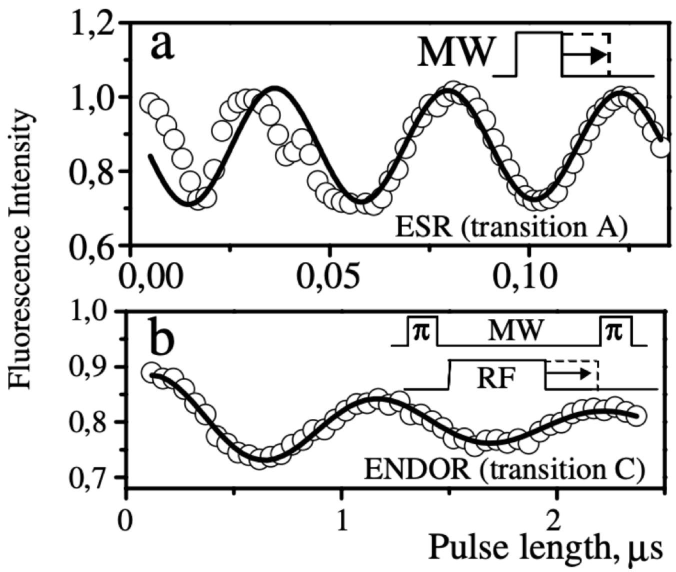
Spin Hamiltonian of NV + nuclear spin

$$H = DS_z^2 + \gamma_e B_0 S_z + \gamma_n B_0 I_z + \vec{S} \cdot \overleftrightarrow{A} \cdot \vec{I}$$

Zero-field splitting — Zeeman for e-spin & n-spin — Hyperfine coupling

secular approximation $\approx H_0 + \gamma_n B_0 I_z + \boldsymbol{A_\parallel S_z I_z} + \frac{A_{aniso}}{2}[S_z I_+ + S_z I_-]$

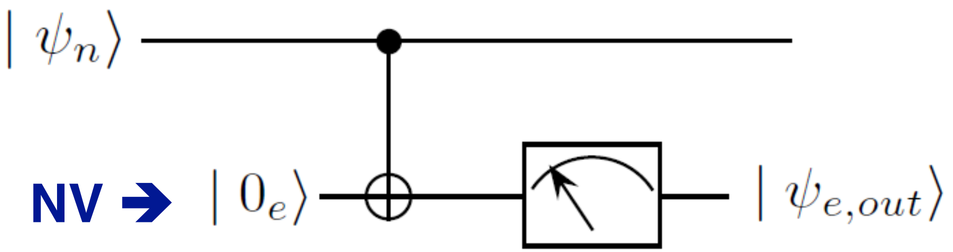


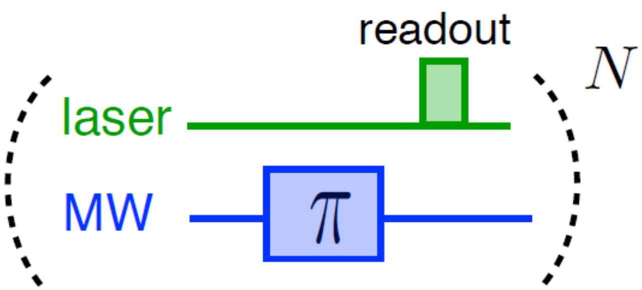


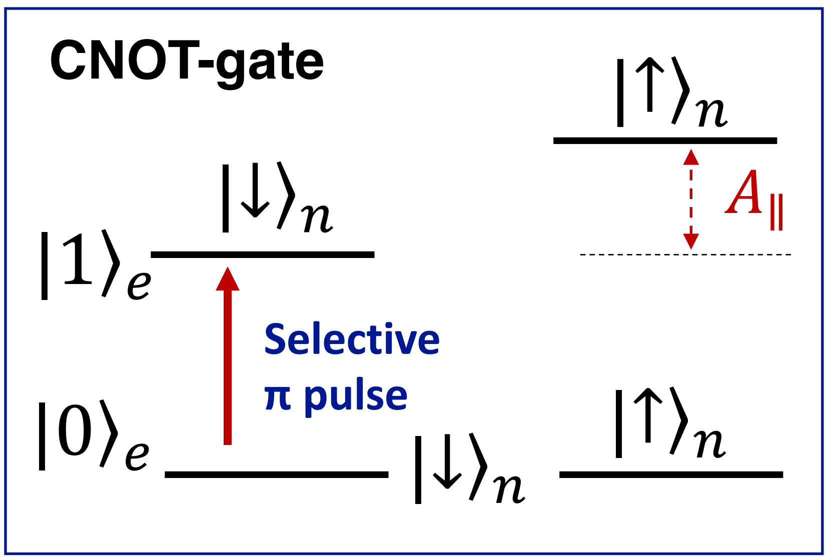
F. Jelezko et al., PRL 93, 130501 (2004).

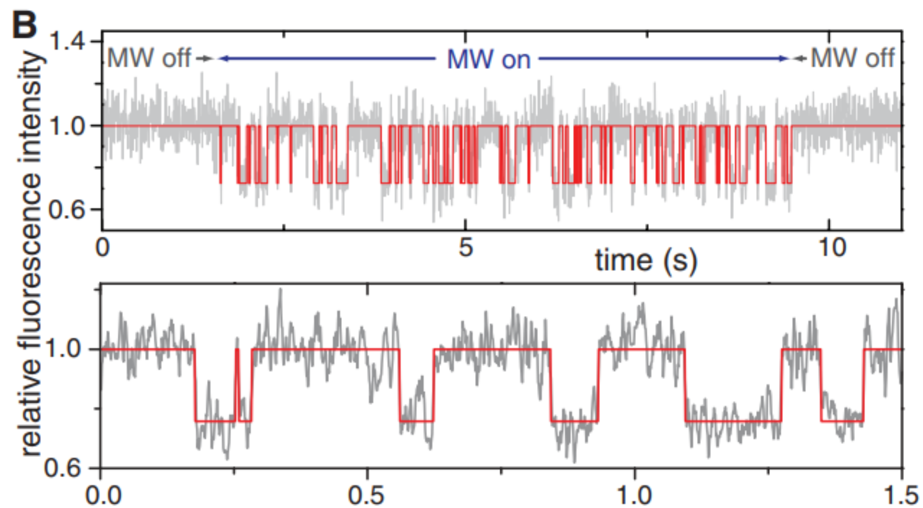
Single-shot readout and preparation

- CNOT gate: flip the NV spin conditional on the n-spin.









P. Neumann et al., Science 329, 542 (2010).

Outline

1. **NV center as a solid-state qubit.**
   - Initialization and readout: Spin-dependent excitation and decay
   - Single-qubit operations via magnetic resonance

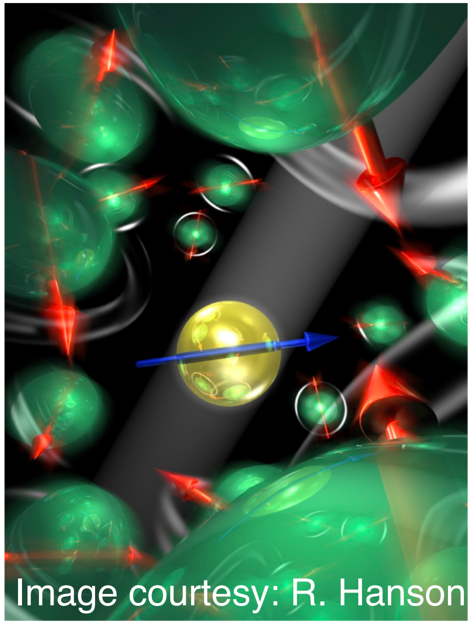
2. **NV – nuclear spin hybrid registers in diamond**
   - Nuclear spins in diamond (^{13}C and ^{14}N)
   - Spin Hamiltonian and 2-qubit gates

3. **Decoherence problem**
   - Qubits are open quantum systems
   - How to protect qubits from decoherence? Echo and dynamical decoupling

4. **Recent advances toward large-scale defect-based quantum computers**

Spin dynamics: Janus aspects of nuclear spins

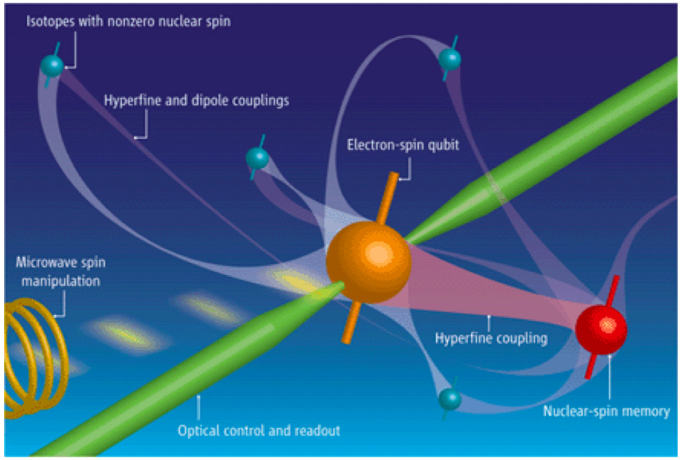
Nuclear spin bath as a cause of quantum decoherence



NV T_2 ~ 0.6 ms (L. M. Pham et al. (2011).)

Isotopic eng. + Dynamical decoupling
➔ T_2 ~ 0.6 sec (N. Bar-Gill et al. (2013).)

Nuclear spin bath as a resource for quantum application



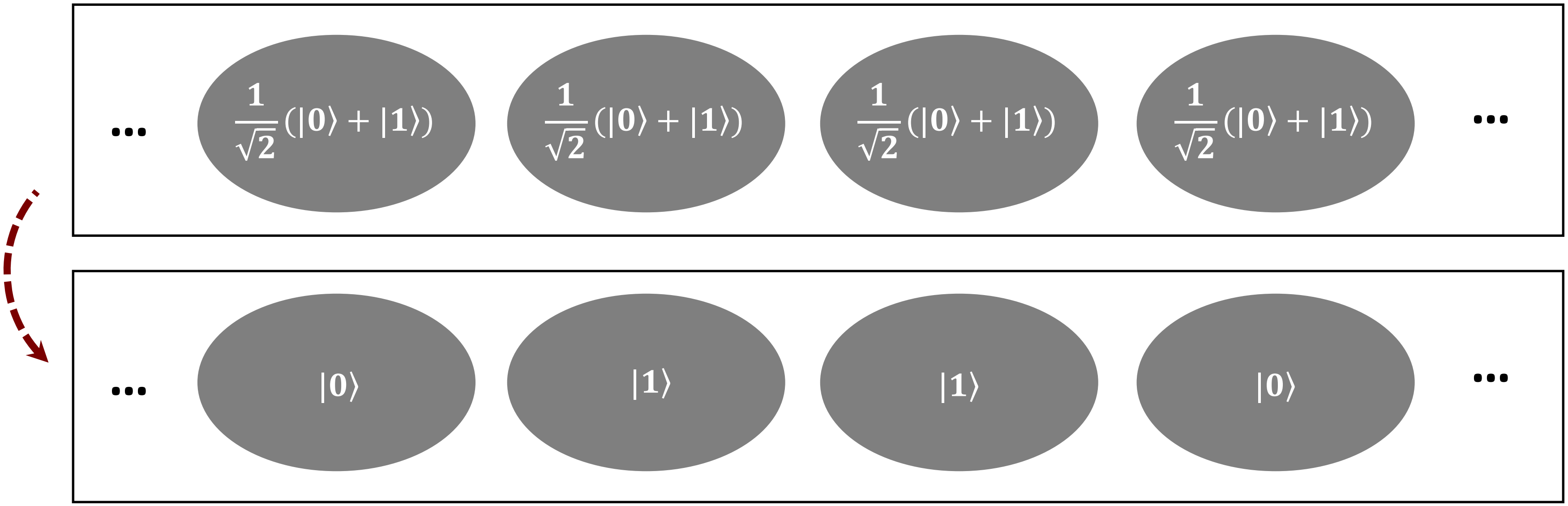
Boehme *et al.*, *Science* (2012)

How to reconcile these two conflicting aspects?

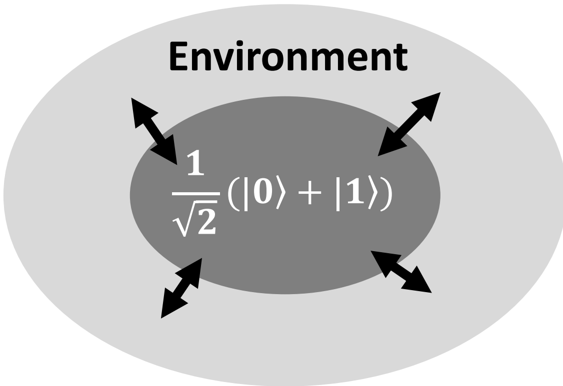
1) Understanding of the decoherence
2) Active protection of the NV coherence

Decoherence of an open quantum system

- **Decoherence is a dynamical transition from a pure quantum state to a classical mixed state.**



- **Decoherence occurs as a result of the interaction with the environment.**



- Thermal noise and magnetic fluctuation
- Magnetic inhomogeneity
  → Relaxation + Dephasing

✓ Interaction with the nuclear spin bath
  → Pure dephasing

Decoherence in terms of density matrix

… $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ …

$$\rho = \sum p_i |\psi_i\rangle\langle\psi_i| = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1| + |0\rangle\langle 1| + |1\rangle\langle 0|) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$tr[\rho^2] = tr[\rho] = 1\ (pure)$$

Decoherence

… $|0\rangle$ $|1\rangle$ $|1\rangle$ $|0\rangle$ …

$$\rho = \sum p_i |\psi_i\rangle\langle\psi_i| = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$tr[\rho^2] = \frac{1}{2} = \frac{1}{N}\ (completely\ mixed)$$

[1] H. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford, 2002)

Decoherence in the Bloch sphere

- In general, for a two-level system $\{|0\rangle, |1\rangle\}$

$$\rho = \frac{1}{2}(\mathbb{I} + r_x\sigma_x + r_y\sigma_y + r_z\sigma_z) = \frac{1}{2}\begin{pmatrix} 1 + r_z & r_x - ir_y \\ r_x + ir_y & 1 - r_z \end{pmatrix}$$

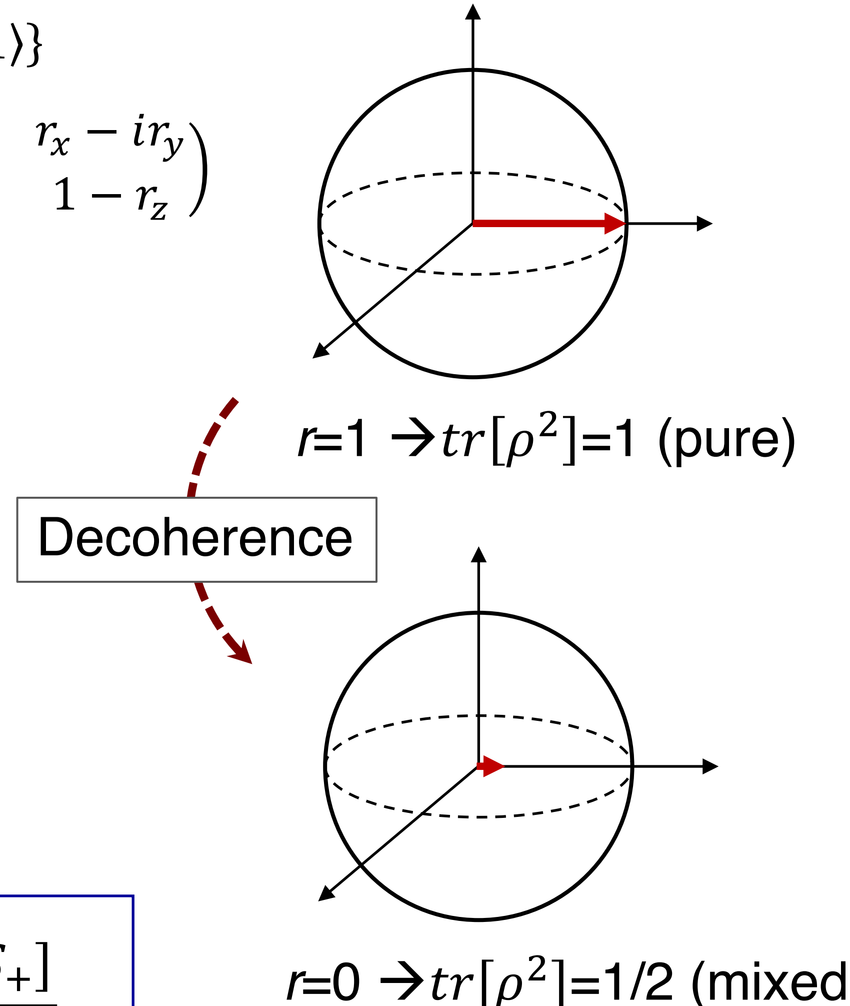
$, where\ r_i = (\sigma_i|\rho) = tr(\rho\sigma_i) =< \sigma_i >$

- Purity: $tr[\rho^2] = \frac{1}{2}(1 + r^2)$

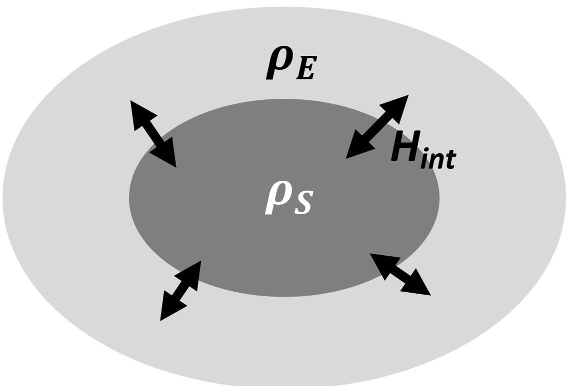
- Coherence function L(t)

$$\rho = \begin{pmatrix} \frac{1}{2}(1 + \langle S_z\rangle) & \langle S_-\rangle \\ \langle S_+\rangle & \frac{1}{2}(1 - \langle S_z\rangle) \end{pmatrix}$$

→Define: $L(t) \equiv \frac{tr[\rho(t)S_+]}{tr[\rho(0)S_+]}$



Let's include the environmental effect.



$H = H_S + H_E + H_{int}$

- Total system as a closed quantum system

$$\rho_{tot}(0) = \rho_s(0) \otimes \rho_E(0)$$

$$\rho_{tot}(t) = U(t)\rho_{tot}(0)U^{\dagger}(t)$$

$$, where\ U(t) = \mathcal{T}_{\leftarrow}\exp[-\frac{i}{\hbar}\int_0^t H(t')dt']$$

- Reduced density matrix[1]: $\rho_s(t) = tr_E[\rho_{tot}(t)]$

$$\langle S_+ \rangle = tr_S[\rho_s(t)S_+] = tr[\rho_{tot}(t)S_+]$$

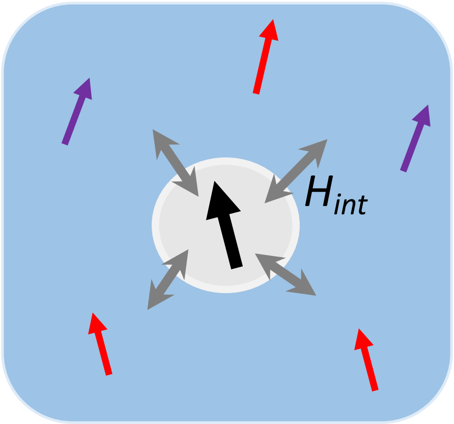
- Coherence function: $L(t) \equiv \dfrac{tr[\rho_{tot}(t)S_+]}{tr[\rho_{tot}(0)S_+]}$

Then, what's the meaning of this?
And how do we calculate it?

[1] Nielsen and Chuang, *Quantum computation and quantum information* (Cambridge, New York, 2000)

Physical meaning of decoherence

1. System + Bath is assumed to be a closed system.



$$H = H_S + H_{Bath} + H_{int}$$
$$= \sum_n |n\rangle\langle n| \otimes B_n$$

2. The total system is initialized at t=0.

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |0\rangle)\otimes|\mathcal{B}(0)\rangle$$

3. The system and the bath are entangled' over time.

$$|\Psi(\tau)\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle\otimes\left|\mathcal{B}^{(0)}(\tau)\right\rangle + |1\rangle\otimes\left|\mathcal{B}^{(1)}(\tau)\right\rangle\right)$$

$$\rho_s = Tr_B[\rho_{total}(\tau)]$$

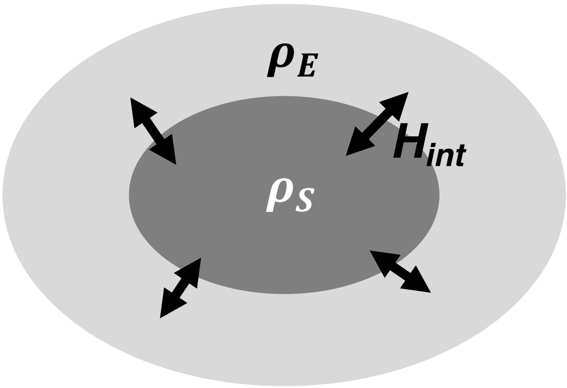
$$= \frac{1}{2}\begin{pmatrix} 1 & \left\langle\mathcal{B}^{(1)}(\tau)\middle|\mathcal{B}^{(0)}(\tau)\right\rangle \\ \left\langle\mathcal{B}^{(0)}(\tau)\middle|\mathcal{B}^{(1)}(\tau)\right\rangle & 1 \end{pmatrix}$$

- *The decoherence is characterized by the bath state overlap [1,2].*

[1] H. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford, 2002)
[2] Nielsen and Chuang, *Quantum computation and quantum information* (Cambridge, New York, 2000)

Two approaches to calculations of quantum decoherence

1. Top-down approach (phenomenological): Lindblad (Markovian) Master Eq.



$$\rho_{tot}(t) \approx \rho_S(t) \otimes \rho_E(t)$$

$$\rho_s \rightarrow \Lambda \rho_s$$

$$\frac{d\rho_s}{dt} = \frac{i}{\hbar}[H, \rho_s] + \sum_{\mu>1} \mathbb{D}[L_\mu]\rho_s$$

2. Bottom-up approach (microscopic): Quantum Bath Approach

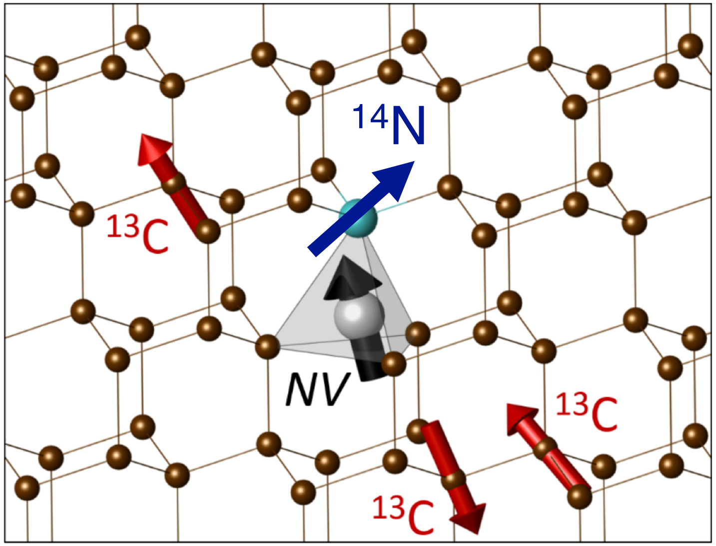
$$\rho_{tot}(t) = U(t)\rho_{tot}(0)U^\dagger(t) \neq \rho_S(t) \otimes \rho_E\ (t) \quad \rightarrow \quad \mathcal{L}(\tau) \equiv \frac{tr[\rho_{tot}(\tau)S_+]}{tr[\rho_{tot}(0)S_+]}$$

Breuer and Petruccione, *The Theory of Open Quantum Systems* (Oxford, 2002)

Quantum bath model for qubit decoherence

Theory: Quantum Bath + Cluster Expansion

*No adjustable free parameters!



***H* = *H*$_{System}$ + *H*$_{Bath}$ + *H*$_{int}$,** where

$$\mathcal{H}_{System} = -\gamma_e \vec{B} \cdot \vec{S} + \Delta S_z^2$$

$$\mathcal{H}_{Bath} = -\vec{B} \cdot \sum_i \gamma_i \vec{I}_i + H_{n-n}$$

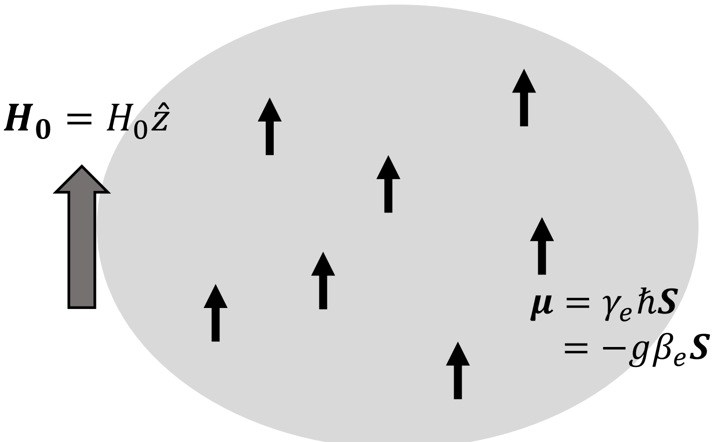
$$\mathcal{H}_{int} = \vec{S} \cdot \sum_i \overleftrightarrow{A}_i \cdot \vec{I}_i$$

J. R. Maze et al., Phys. Rev. B **78**, 094303 (2008).
N. Zhao et al., Phys. Rev. B **85**, 115303 (2012).
H. Seo et al., Nat. Comm. **7**, 12935 (2016)

$$\rho_{tot}(t) = U(t)\rho_{tot}(0)U^{\dagger}(t)$$

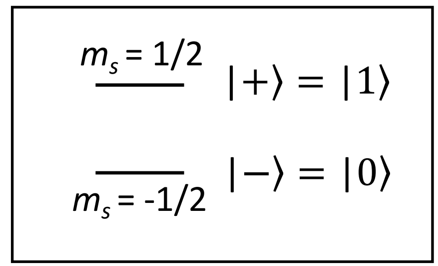
Magnetic resonance: rotating frame

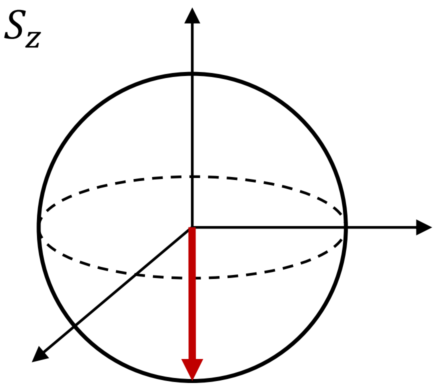
- **Consider a collection of S=1/2 spin-moments under a static B-field**



$$\mathcal{H} = -\boldsymbol{\mu}\cdot\boldsymbol{H_0} = -\hbar(\gamma_e H_0)S_z = \hbar w_e S_z$$

*Note: γ_e <0





$$\rho = |0\rangle\langle 0|$$

- **Apply :** $H_x \cos wt\, \hat{x} = \boldsymbol{H_R} + \boldsymbol{H_L}$

$$\mathcal{H} = \hbar w_e S_z - \hbar\gamma_e H_1\left(S_x \cos wt + S_y \sin wt\right) = \hbar w_e S_z - \hbar\gamma_e H_1(e^{-iwtS_z} S_x e^{iwtS_z})$$

$$\frac{d\rho}{dt} = \frac{i}{\hbar}[\rho, \mathcal{H}(t)] \longrightarrow \frac{d\rho_R}{dt} = \frac{i}{\hbar}[\rho_R, \mathcal{H}_{eff}]$$,where $\rho_R = R^{-1}\rho R$

Rotating frame

$$\psi = e^{-iwtS_z}\psi_R = R\psi_R$$

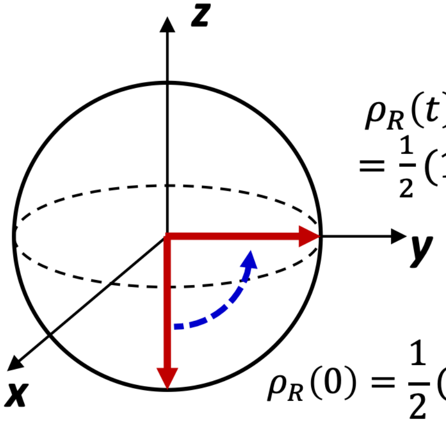
$$\mathcal{H}_{eff} = \hbar(w_e - w)S_z - \gamma_e \hbar H_1 S_x$$

The time dependence is removed.

Decoherence: Quantum bath model

- **Resonance at $w = w_e$ → The spin will precess in the *yz*-plane in the rotating frame**

$$\mathcal{H}_{eff} = \hbar(w_e - w)S_z - \gamma_e \hbar H_1 S_x = \hbar w_1 S_x$$



$$\rho_R(t) = U(t)\rho_R(0)U^\dagger(t)$$
$$= \frac{1}{2}(1 + \sigma_y \sin w_1 t - \sigma_z \cos w_1 t)$$

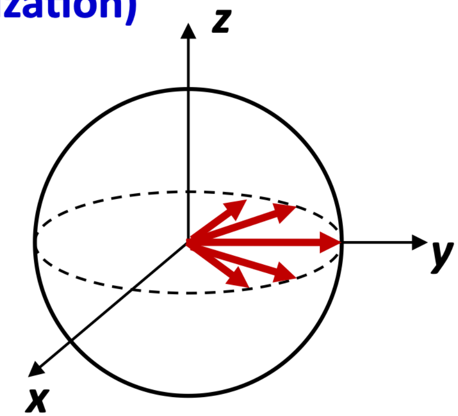
$w_1 t = \pi/2$ →

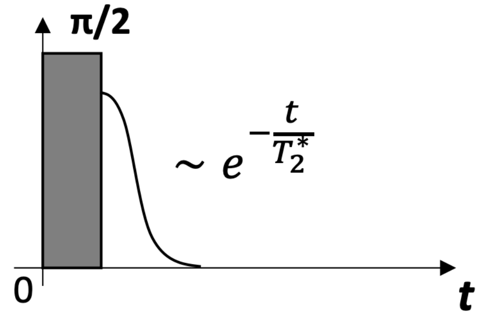
$$\rho_R\left(\frac{\pi}{2}\right) = \frac{1}{2}(1 + \sigma_y) = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$$

Coherence is created.

$$\rho_R(0) = \frac{1}{2}(1 - \sigma_z)$$

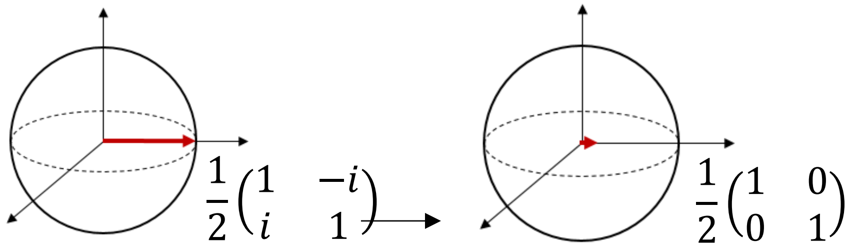
- **π/2 pulse + magnetic inhomogeneity = Free induction decay (*loss of the transverse magnetization)**



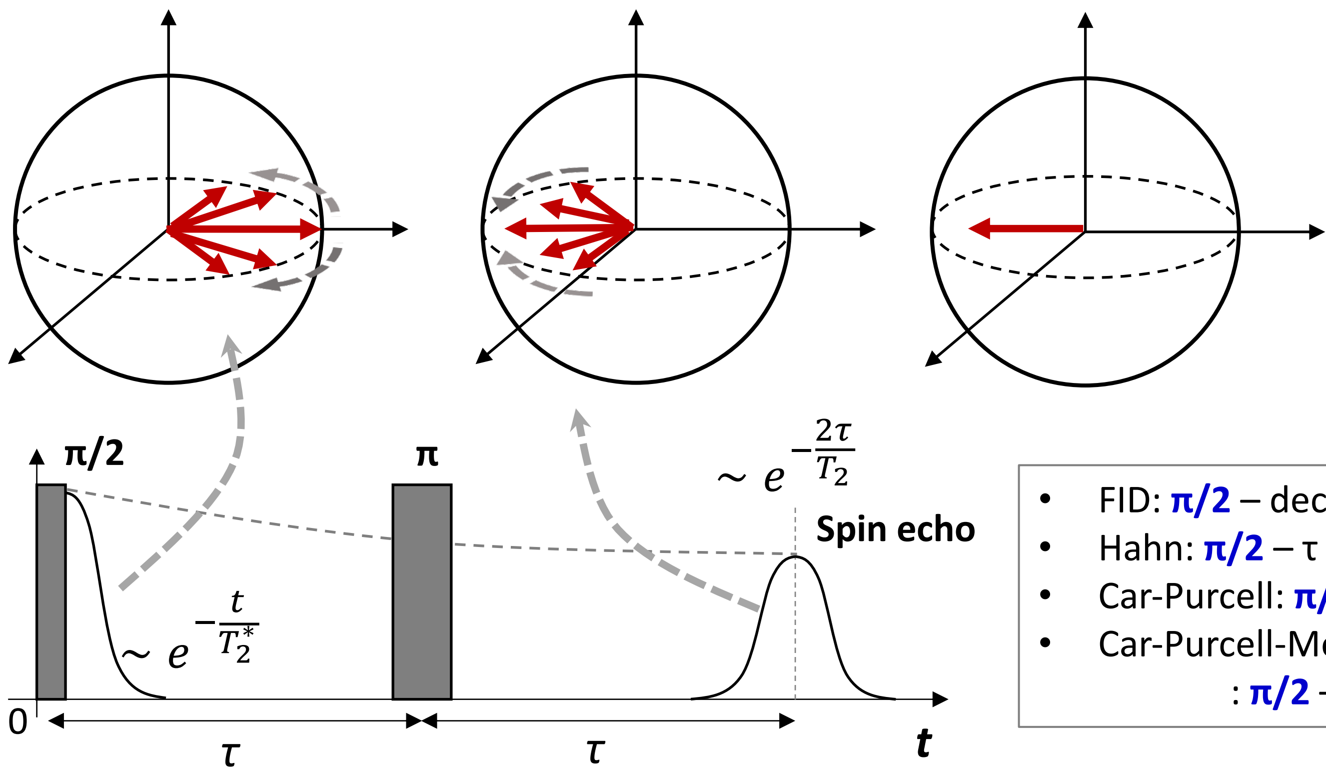


Decoherence: Quantum bath model

- **But, we are interested in the pure dephasing.**



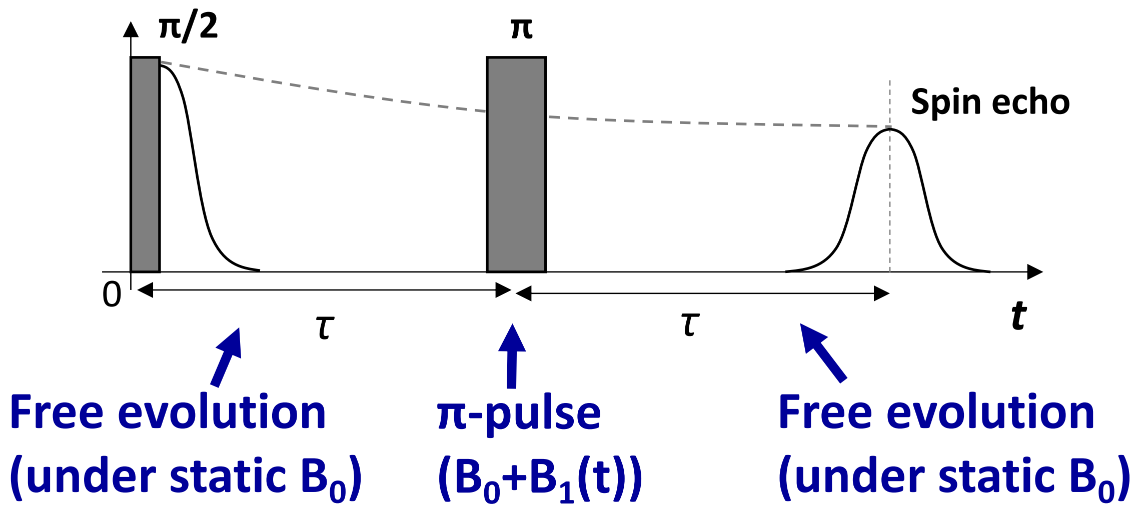
- **Flip the spin using a π-pulse**



- FID: **π/2** – decay
- Hahn: **π/2** – τ – **π** – τ - echo
- Car-Purcell: **π/2** – τ – **π_x** – 2τ – **π_x** …
- Car-Purcell-Meiboom-Gill (CPMG)
  : **π/2** – τ – **π_y** – 2τ – **π_y** …

Decoherence: Quantum bath model

- Let's construct the propagator U(t) for the Hahn-echo sequence.



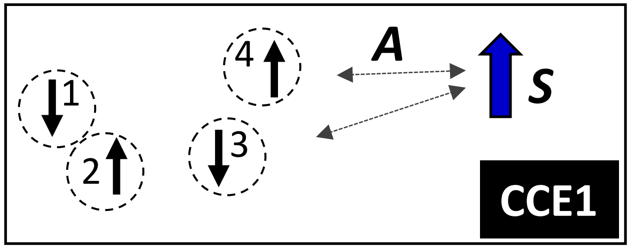
$$\mathcal{L}(\tau) = tr[\rho_{tot}(t)S_+], where \;\; \rho_{Bath}(0) = \sum \mathcal{P}_\mathcal{J}|\mathcal{J}\rangle\langle\mathcal{J}|$$

$$\mathcal{L}(\tau) = \sum_{\mathcal{J}} \mathcal{P}_\mathcal{J} \langle\mathcal{J}|\mathcal{U}_-^\dagger\mathcal{U}_+^\dagger\mathcal{U}_-\mathcal{U}_+|\mathcal{J}\rangle$$

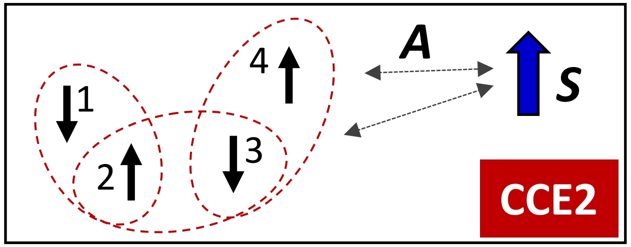
Decoherence: Quantum bath model

- For R_{bath} = 5 nm: # of n-spins ~ 1000 ➔ *D*(Hamiltonian) = 2^{1500}
- Use the cluster-correlation expansion method [1].

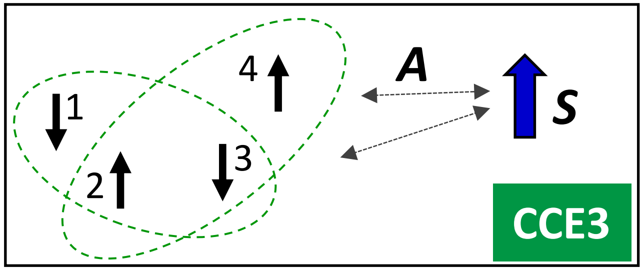
$$\mathcal{L}_1(\tau) = \prod_i \tilde{\mathcal{L}}_i(\tau) = \prod_i \mathcal{L}_i(\tau) / \tilde{\mathcal{L}}_0$$



$$\mathcal{L}_2(\tau) = \prod_i \tilde{\mathcal{L}}_i(\tau) \prod_{\{i,j\}} \tilde{\mathcal{L}}_{i,j} \qquad \tilde{\mathcal{L}}_{i,j} = \frac{\mathcal{L}_{i,j}(\tau)}{\tilde{\mathcal{L}}_i \tilde{\mathcal{L}}_j}$$



$$\mathcal{L}_3(\tau) = \prod_i \tilde{\mathcal{L}}_i(\tau) \prod_{\{i,j\}} \tilde{\mathcal{L}}_{i,j} \prod_{\{i,j,k\}} \tilde{\mathcal{L}}_{i,j,k}$$

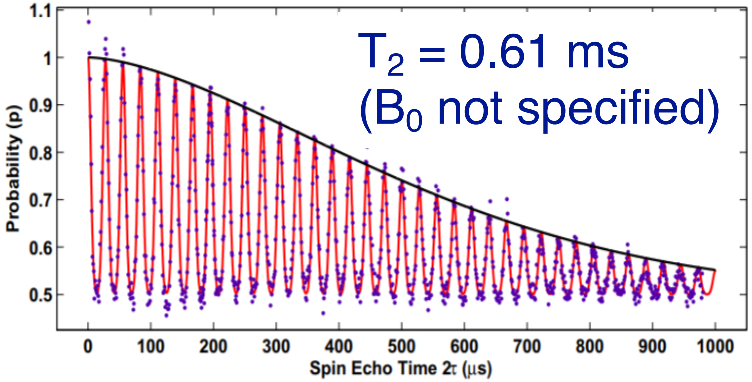


$$\mathcal{L}_N(\tau) = \prod_{C \subseteq \{1,2,3,\ldots,N\}} \tilde{\mathcal{L}}_C(\tau)$$

W Yang and RB Liu, *Quantum many-body theory of qubit decoherence in a finite-size spin bath*, PRB **78**, 085315 (2008)

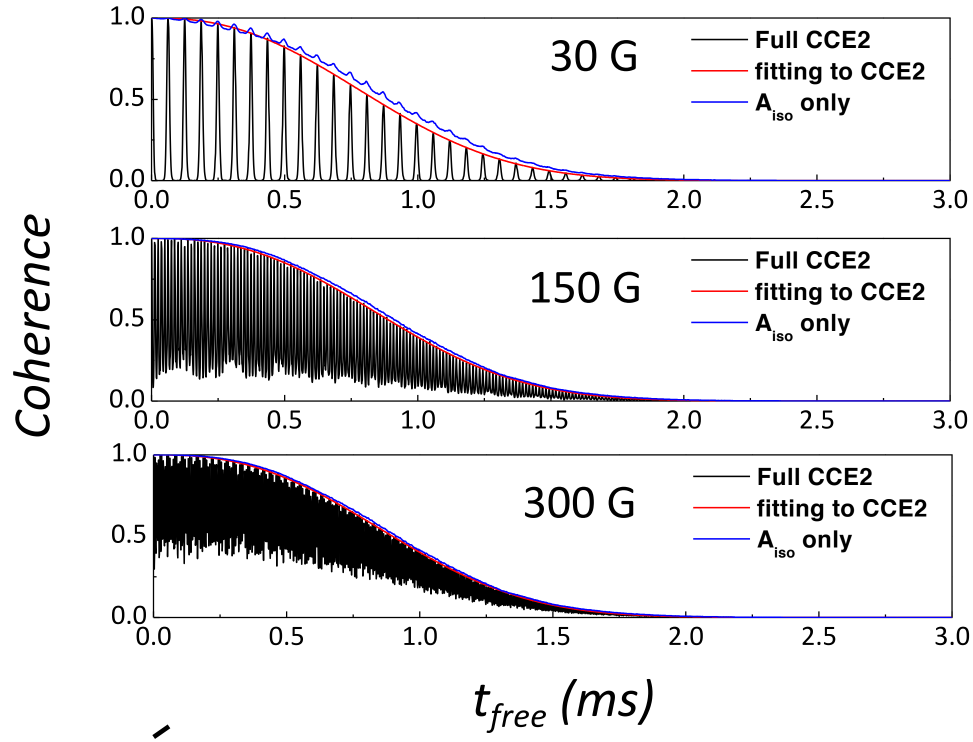
Finally, the Hahn-echo decoherence of NV

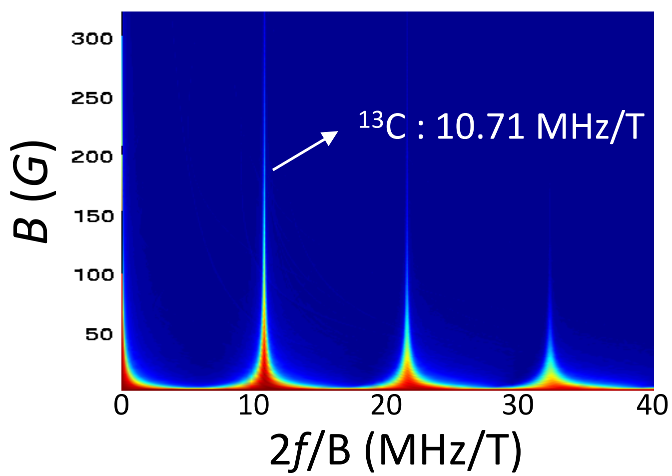
Experiment



L. M. Pham et al., New J. Phys. **13,** 045021 (2011).

Theory (CCE2)





B-normalized FFT spectrum

T_2 = 0.76 ms
(theoretical limit)

Outline

1. **NV center as a solid-state qubit.**
   - Initialization and readout: Spin-dependent excitation and decay
   - Single-qubit operations via magnetic resonance

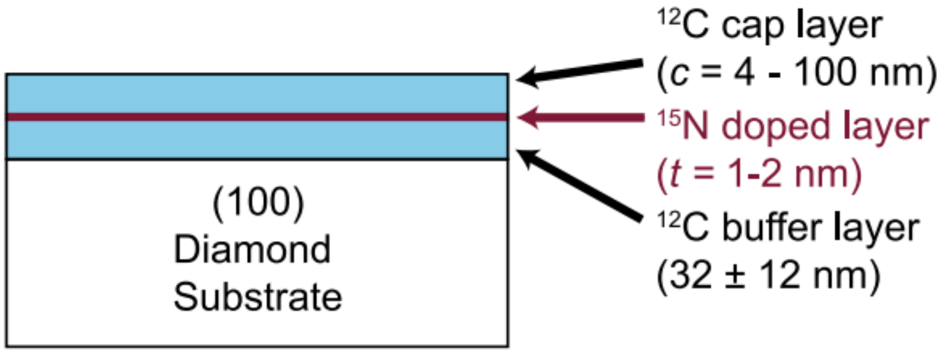
2. **NV – nuclear spin hybrid registers in diamond**
   - Nuclear spins in diamond (^{13}C and ^{14}N)
   - Spin Hamiltonian and 2-qubit gates

3. **Decoherence problem**
   - Qubits are open quantum systems
   - How to protect qubits from decoherence? Echo and dynamical decoupling

4. **Recent advances toward large-scale defect-based quantum computers**

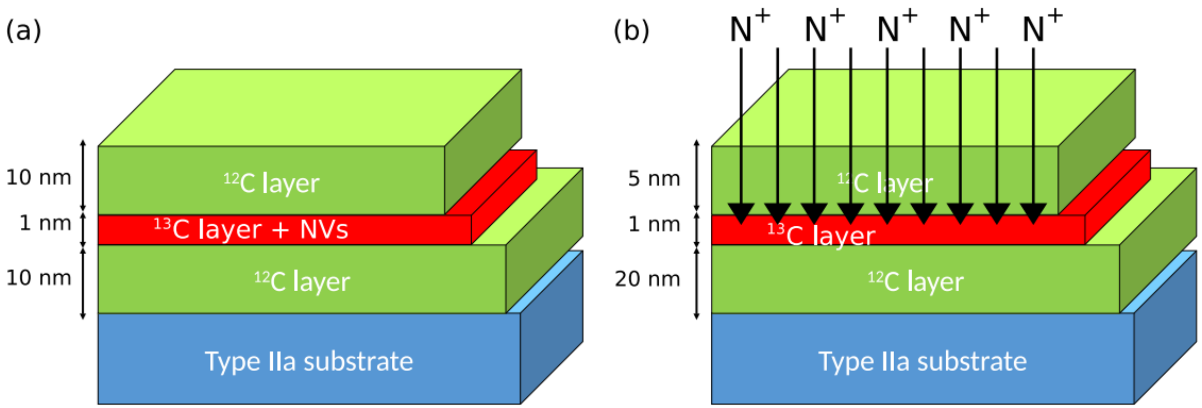
Deterministic implantation of NV centers

- **Depth control: delta-doped CVD growth**



K. Ohno et al., APL **101**, 082413 (2012)

- **Depth and thickness control of NV-nuclear spin hybrid registers**

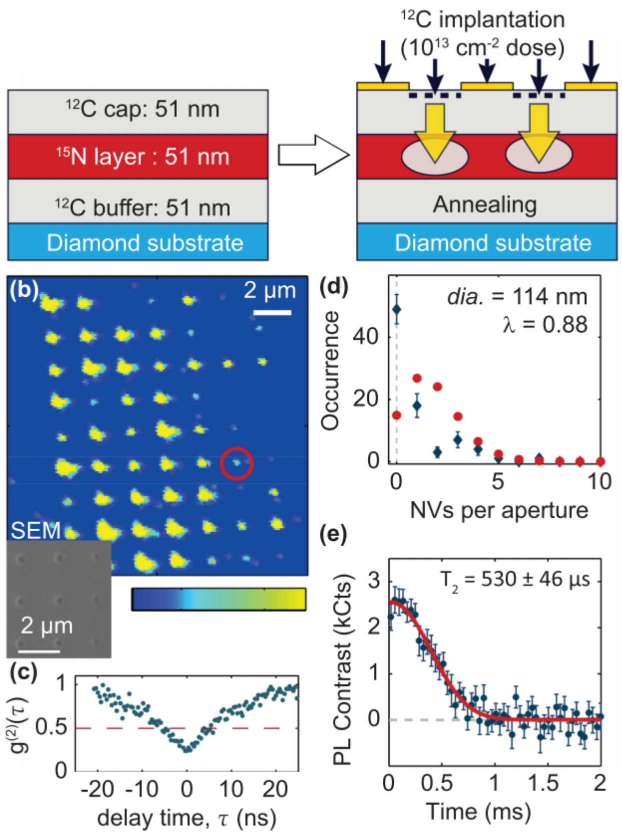


T. Unden et al., npj Quantum Info. **4**, 39 (2018).

Deterministic implantation of NV centers

- **Lateral control**

Masked implantation



K. Ohno et al., APL **105**, 052406 (2014)

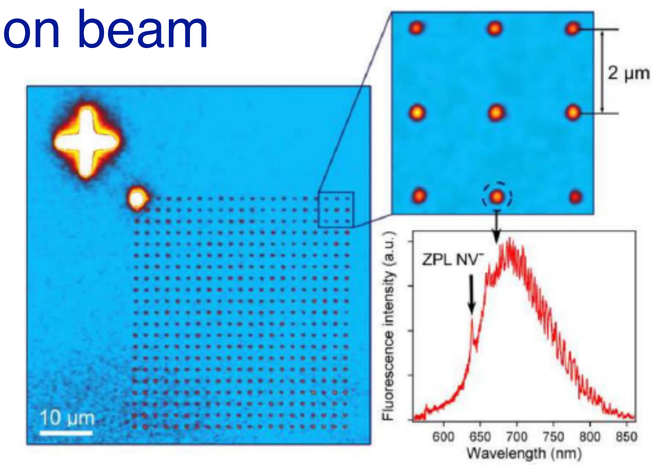
Recent review

APL PHOTONICS **1**, 020801 (2016)

Invited Article: Precision nanoimplantation of nitrogen vacancy centers into diamond photonic crystal cavities and waveguides

M. Schukraft,[1,2,a,b] J. Zheng,[1,3,a] T. Schröder,[1] S. L. Mouradian,[1] M. Walsh,[1] M. E. Trusheim,[1] H. Bakhru,[4] and D. R. Englund[1,c]

Focused ion beam



M. Lesik et al., PSSA 210, 2055 (2013)

Toward large-scale quantum computers

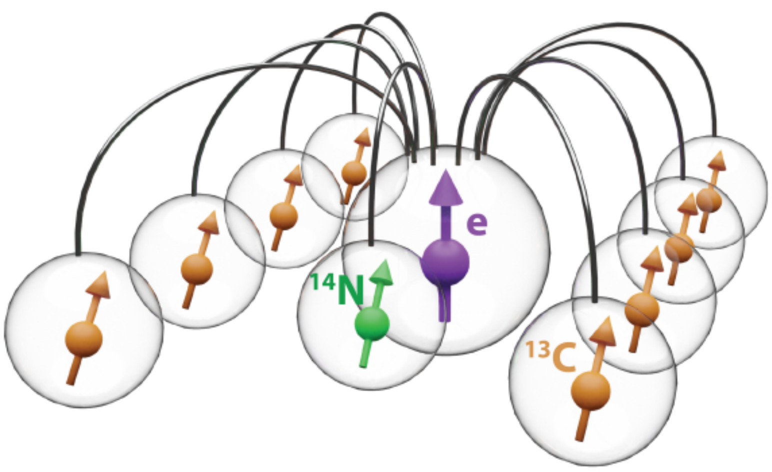
A 10-qubit solid-state spin register with quantum memory up to one minute

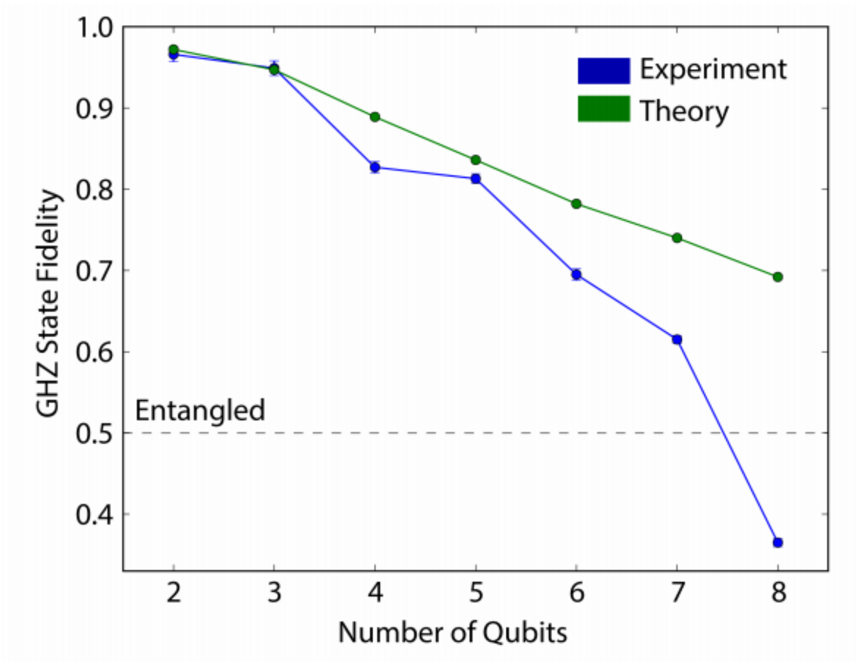
C. E. Bradley[1,2],* J. Randall[1,2],* M. H. Abobeih[1,2], R. C. Berrevoets[1,2], M. J. Degen[1,2], M. A. Bakker[1,2], M. Markham[3], D. J. Twitchen[3], and T. H. Taminiau[1,2†]

[1] *QuTech, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands*
[2] *Kavli Institute of Nanoscience Delft, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands and*
[3] *Element Six, Fermi Avenue, Harwell Oxford, Didcot, Oxfordshire, OX11 0QR, United Kingdom*

arXiv:1905.02094

(Dated: May 7, 2019)





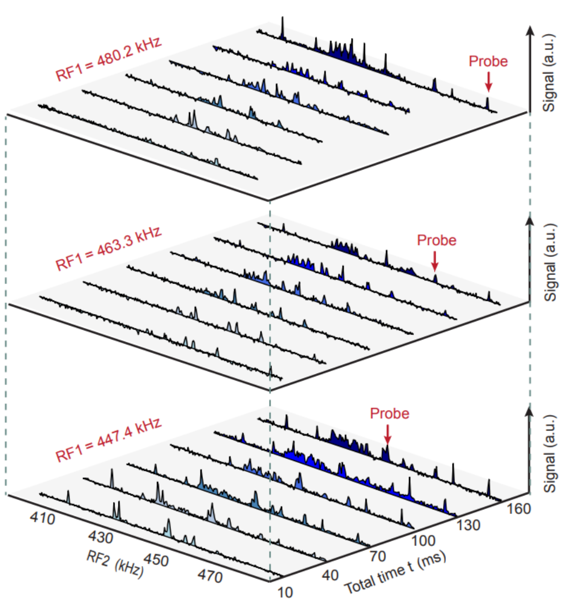
Toward large-scale quantum computers

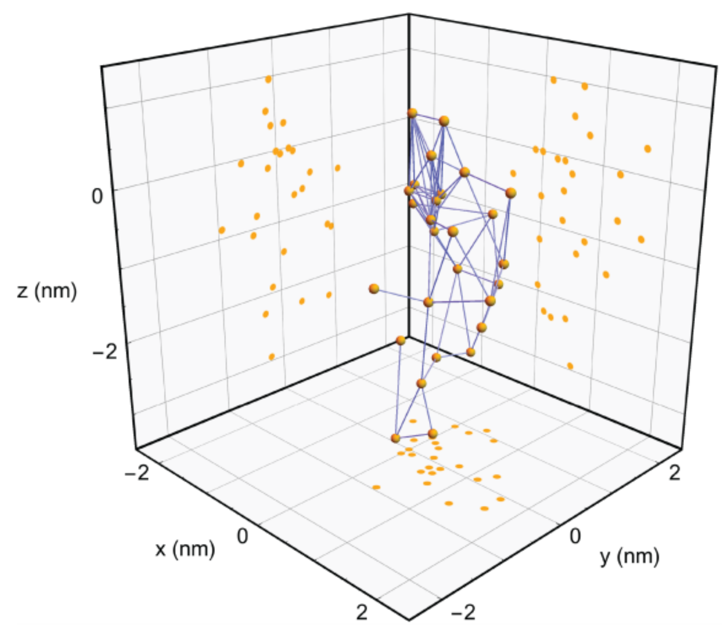
Atomic-scale imaging of a 27-nuclear-spin cluster using a single-spin quantum sensor

M. H. Abobeih[1,2], J. Randall[1,2], C. E. Bradley[1,2], H. P. Bartling[1,2], M. A. Bakker[1,2], M. J. Degen[1,2], M. Markham[3], D. J. Twitchen[3], and T. H. Taminiau[1,2*]
[1] *QuTech, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands*
[2] *Kavli Institute of Nanoscience Delft, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands and*
[3] *Element Six, Fermi Avenue, Harwell Oxford, Didcot, Oxfordshire, OX11 0QR, United Kingdom*

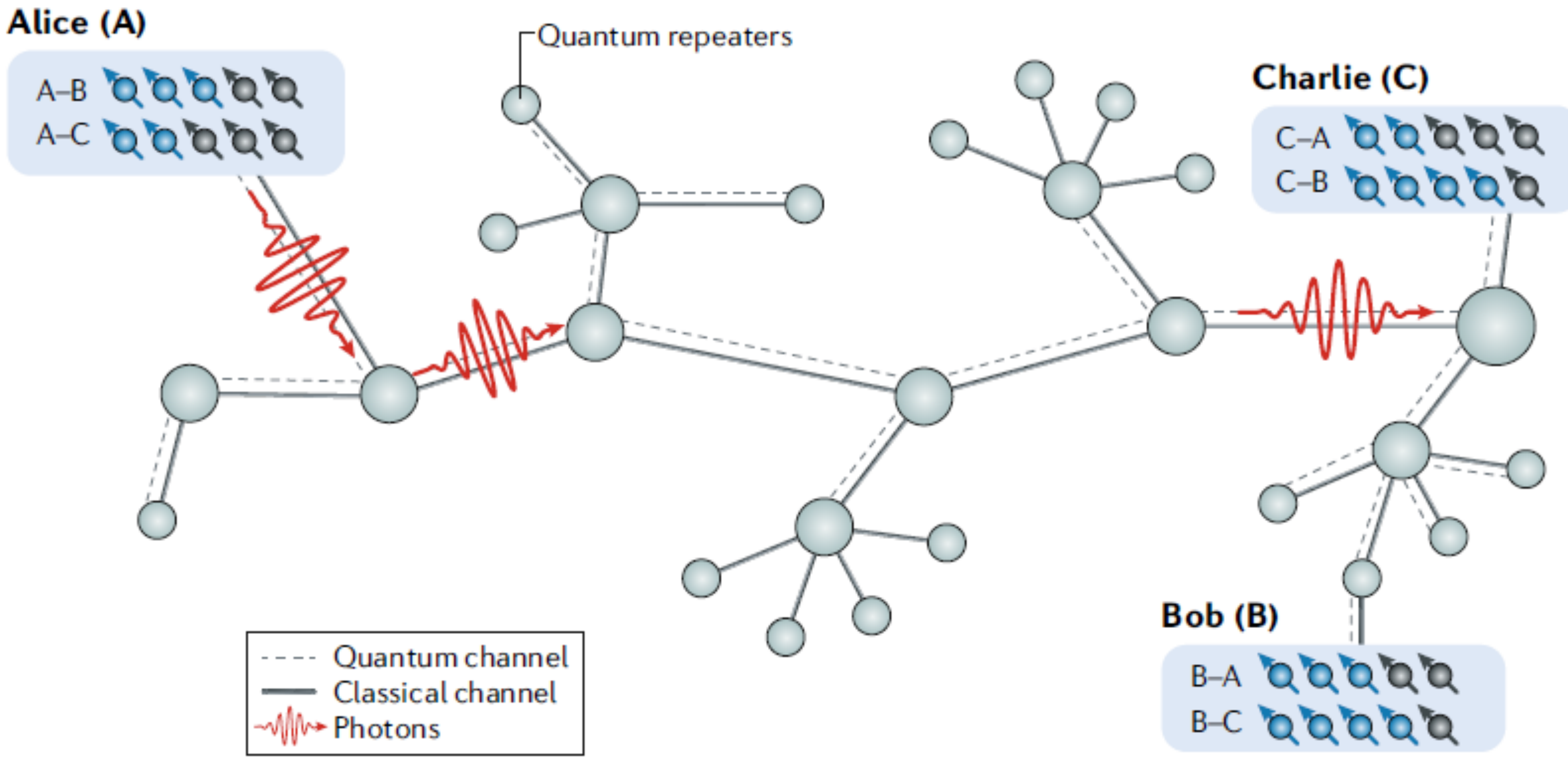
(Dated: May 13, 2019)

arXiv:1905.02095





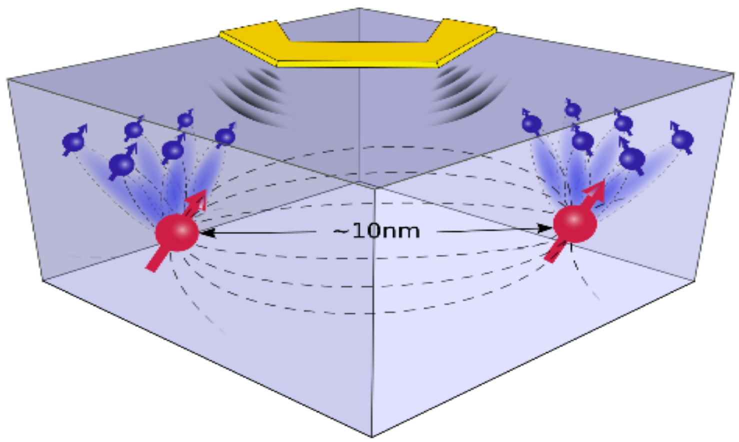
Modular design: distributed quantum computing



M. Atatüre, D. Englund, N. Vamivakas, S.-Y. Lee, & J. Wrachtrup, Nat. Rev. Mater. 3, 38–51 (2018).

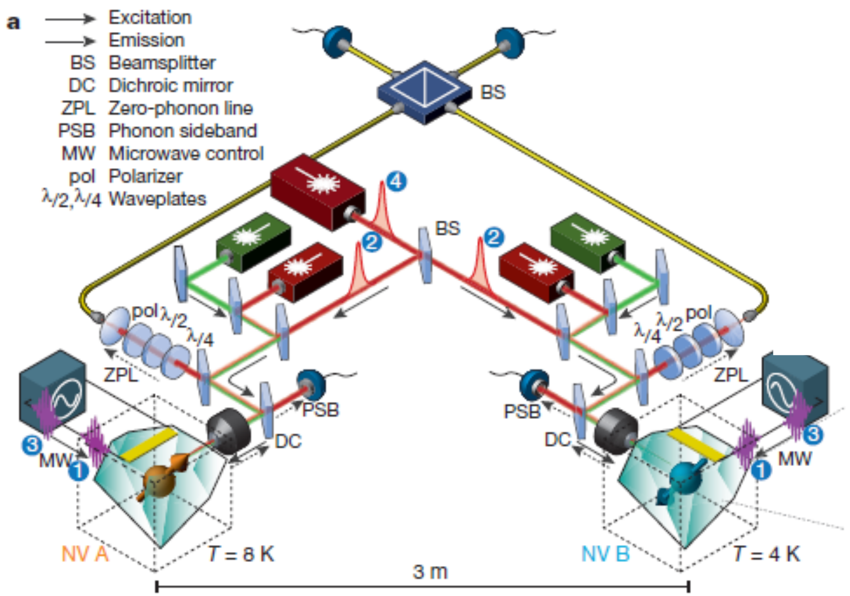
Connecting qubits: spin-spin & spin-to-photon

Dipolar electron spin-spin interaction



Dolde et al., Nature Phys. **9**, 139 (2013)

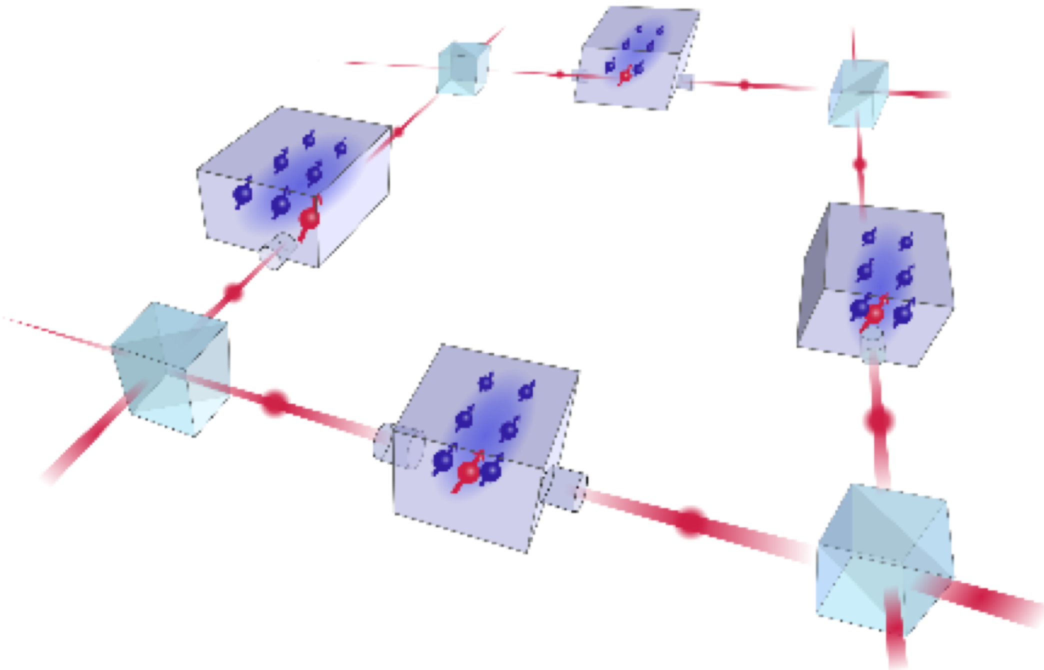
Photon-mediated remote entanglement

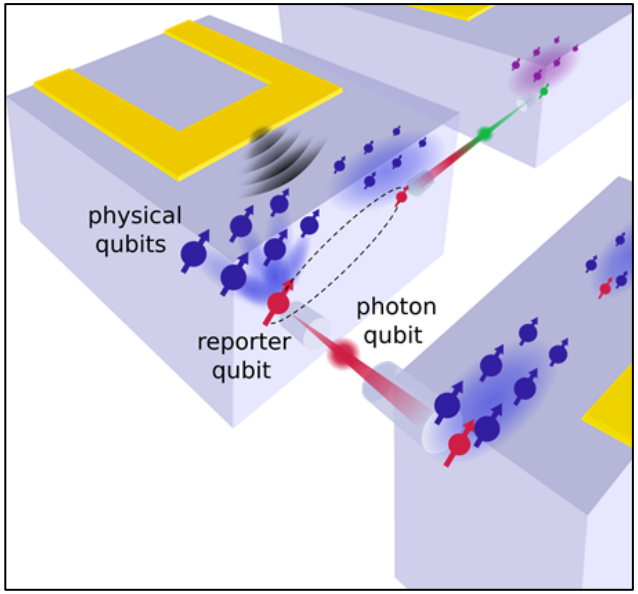


Bernien et al., Nature **497**, 86 (2013)

Potentially, the followings may play a key role as well: phonon, strain, spin-waves. For example, see Whiteley et al., Nature Phys. **15**, 490 (2019).

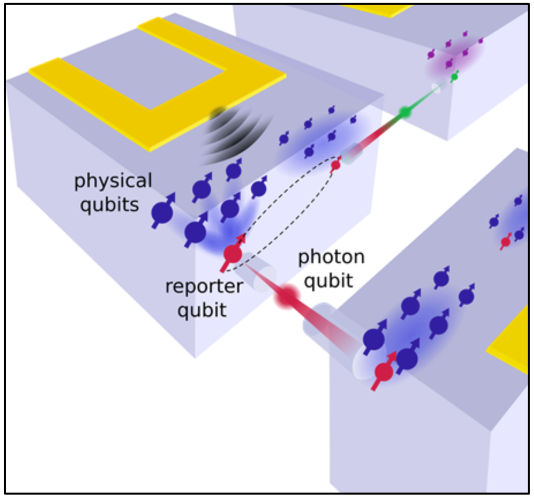
Modular design for quantum computing





Outline

1. **NV center as a solid-state qubit.**
   - Initialization and readout: Spin-dependent excitation and decay
   - Single-qubit operations via magnetic resonance



2. **NV – nuclear spin hybrid registers in diamond**
   - Nuclear spins in diamond (^{13}C and ^{14}N)
   - Spin Hamiltonian and 2-qubit gates

3. **Decoherence problem**
   - Qubits are open quantum systems
   - How to protect qubits from decoherence? Echo and dynamical decoupling

4. **Recent advances toward large-scale defect-based quantum computers**