

# AMAZING POINT DEFECTS OR HÄMMÄSTYTTÄVIÄ PISTEVIRHEITÄ

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Research Group*

# Outline

## Part I.

- Q & A = 🤖

## Part II.

### Theory of the NV center

- Structure
- Electronic structure
- Spin
- Optical properties
- ODMR
- Coherence and spin manipulation

## Part III.

- Interesting experiments and papers
- Perspectives and challenges in QC and QRC

# PART I.

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Q & A

# What is the highest temperature at which coherent quantum control has been carried out?

## Quantum Coherence Control at Temperatures up to 1400 K

Jing-Wei Fan,<sup>○</sup> Shuai-Wei Guo,<sup>○</sup> Chao Lin, Ning Wang, Gang-Qin Liu, Quan Li,<sup>\*</sup> and Ren-Bao Liu<sup>\*</sup>



Cite This: <https://doi.org/10.1021/acs.nanolett.4c04359>



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Metrics & More

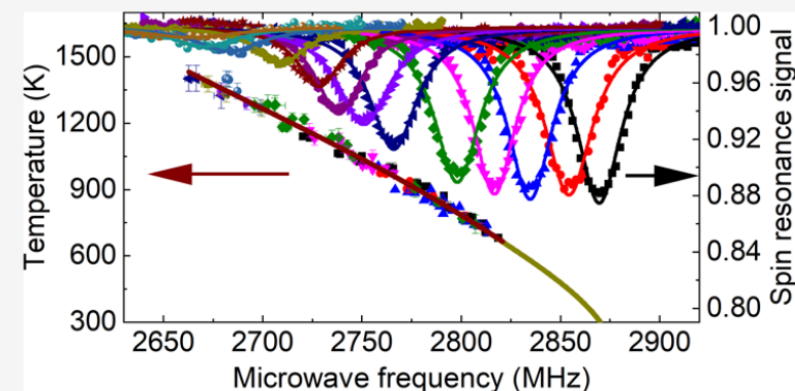


Article Recommendations



Supporting Information

**ABSTRACT:** Coherent quantum control at high temperatures is important for expanding the quantum world and is useful for applying quantum technologies to realistic environments. Quantum control of spins in diamond has been demonstrated near 1000 K, with the spins polarized and read out at room temperature and controlled at elevated temperatures by rapid heating and cooling. Further increase of the working temperature is challenging due to fast spin relaxation in comparison with the heating and cooling rates. Here we significantly improve the heating and cooling rates by using reduced graphene oxide as the laser absorber and heat drain and hence realize coherent quantum operation at up to 1400 K, which is higher than the Curie temperatures of all known materials. This work facilitates the use of diamond sensors to study



# Is it possible to observe quantum jumps of a **single** nuclear spin?

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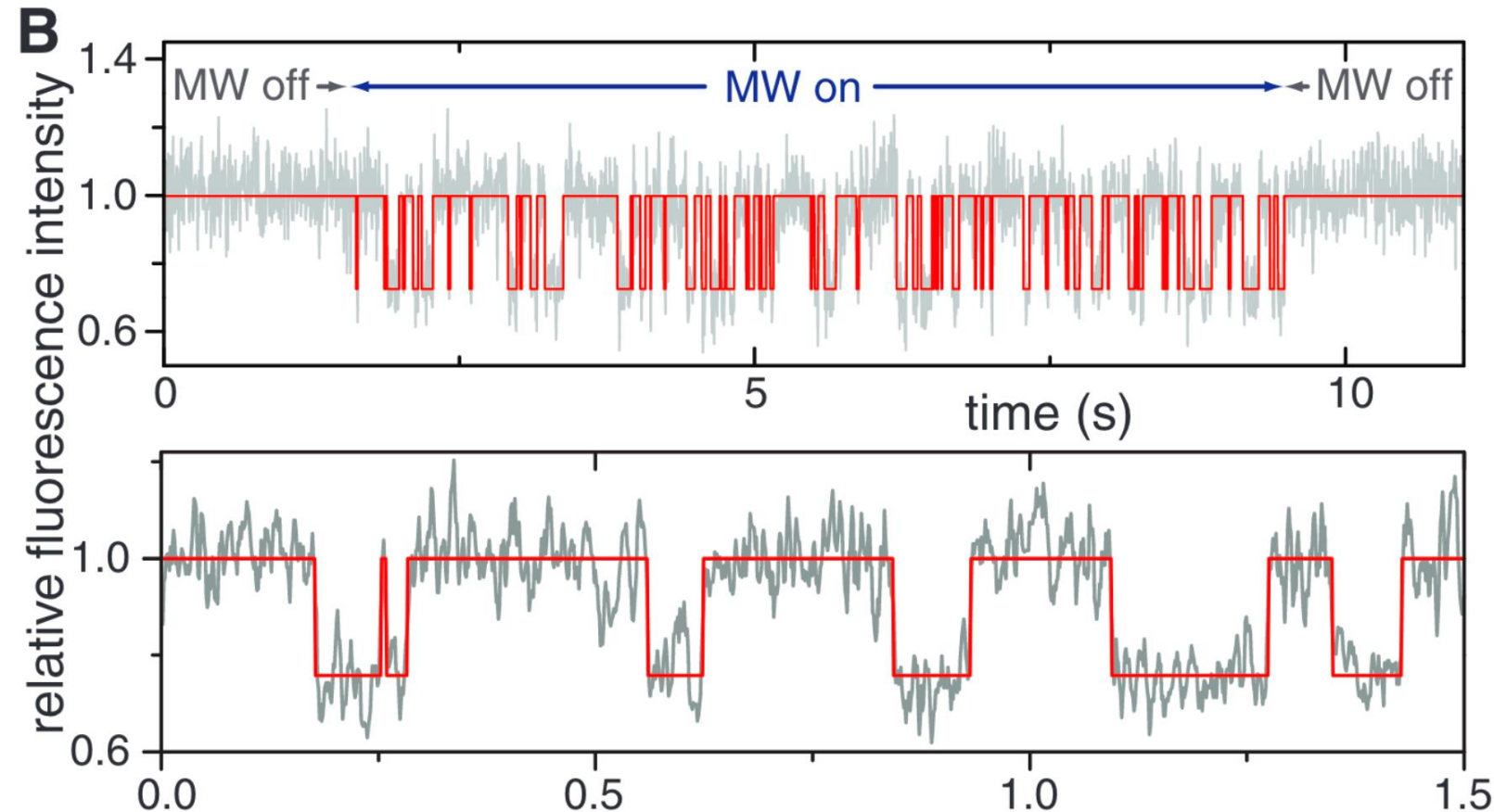
HOME > SCIENCE > VOL. 329, NO. 5991 > SINGLE-SHOT REA

REPORT

## Single-Shot Readout o

PHILIPP NEUMANN, JOHANNES BECK, MATTHIAS STEINER, FLORIAN R

[Affiliations](#)



# What is the longest quantum memory in solids at room temperature?

PHYSICAL REVIEW X **9**, 031045 (2019)

Featured in Physics

## A Ten-Qubit Solid-State Spin Register with Quantum Memory up to One Minute

C. E. Bradley,<sup>1,2,†</sup> J. Randall,<sup>1,2,†</sup> M. H. Abobeih,<sup>1,2</sup> R. C. Berrevoets,<sup>1,2</sup> M. J. Degen,<sup>1,2</sup>  
M. A. Bakker,<sup>1,2</sup> M. Markham,<sup>3</sup> D. J. Twitchen,<sup>3</sup> and T. H. Taminiau<sup>1,2,\*</sup>

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(Received 9 May 2019; published 11 September 2019)

Is the collapse of the wavefunction of entangled particles limited by the speed of light?

# LETTER

doi:10.1038/nature15759

## Loophole-free Bell inequality violation using electron spins separated by 1.3 kilometres

B. Hensen<sup>1,2</sup>, H. Bernien<sup>1,2†</sup>, A. E. Dréau<sup>1,2</sup>, A. Reiserer<sup>1,2</sup>, N. Kalb<sup>1,2</sup>, M. S. Blok<sup>1,2</sup>, J. Ruitenber<sup>1,2</sup>, R. F. L. Vermeulen<sup>1,2</sup>, R. N. Schouten<sup>1,2</sup>, C. Abellán<sup>3</sup>, W. Amaya<sup>3</sup>, V. Pruneri<sup>3,4</sup>, M. W. Mitchell<sup>3,4</sup>, M. Markham<sup>5</sup>, D. J. Twitchen<sup>5</sup>, D. Elkouss<sup>1</sup>, S. Wehner<sup>1</sup>, T. H. Taminiau<sup>1,2</sup> & R. Hanson<sup>1,2</sup>

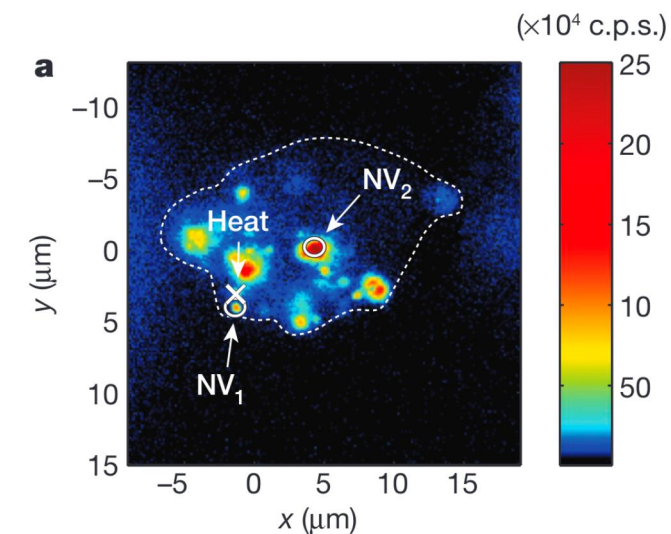
# Can we measure temperature in living cells?

## LETTER

doi:10.1038/nature12373

## Nanometre-scale thermometry in a living cell

G. Kucsko<sup>1\*</sup>, P. C. Maurer<sup>1\*</sup>, N. Y. Yao<sup>1</sup>, M. Kubo<sup>2</sup>, H. J. Noh<sup>3</sup>, P. K. Lo<sup>4</sup>, H. Park<sup>1,2,3</sup> & M. D. Lukin<sup>1</sup>



# What is the frequency resolution of nanoscale sensors?

## REPORT

### QUANTUM MEASUREMENT

## Submillihertz magnetic spectroscopy performed with a nanoscale quantum sensor

Simon Schmitt,<sup>1</sup> Tuvia Gefen,<sup>2</sup> Felix M. Stürner,<sup>1</sup> Thomas Uden,<sup>1</sup> Gerhard Wolff,<sup>1</sup> Christoph Müller,<sup>1</sup> Jochen Scheuer,<sup>1,3</sup> Boris Naydenov,<sup>1,3</sup> Matthew Markham,<sup>4</sup> Sebastien Pezzagna,<sup>5</sup> Jan Meijer,<sup>5</sup> Ilai Schwarz,<sup>3,6</sup> Martin Plenio,<sup>3,6</sup> Alex Retzker,<sup>2</sup> Liam P. McGuinness,<sup>1\*</sup> Fedor Jelezko<sup>1,3</sup>

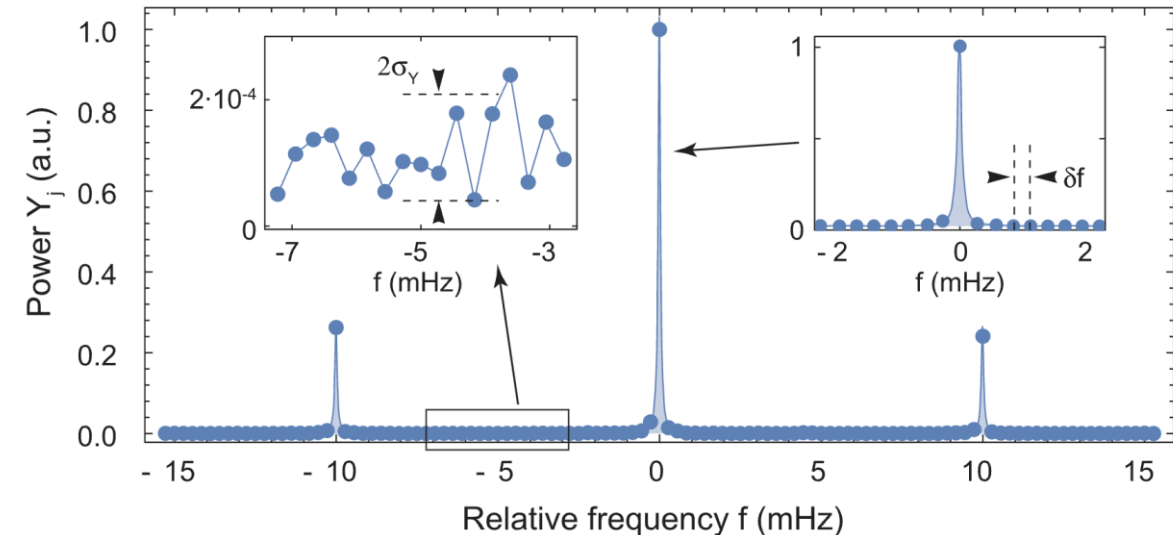
*Science* **356**, 832–837 (2017)

*Science* **356**, 837–840 (2017)

### QUANTUM MEASUREMENT

## Quantum sensing with arbitrary frequency resolution

J. M. Boss,<sup>\*</sup> K. S. Cujia,<sup>\*</sup> J. Zopes, C. L. Degen<sup>†</sup>



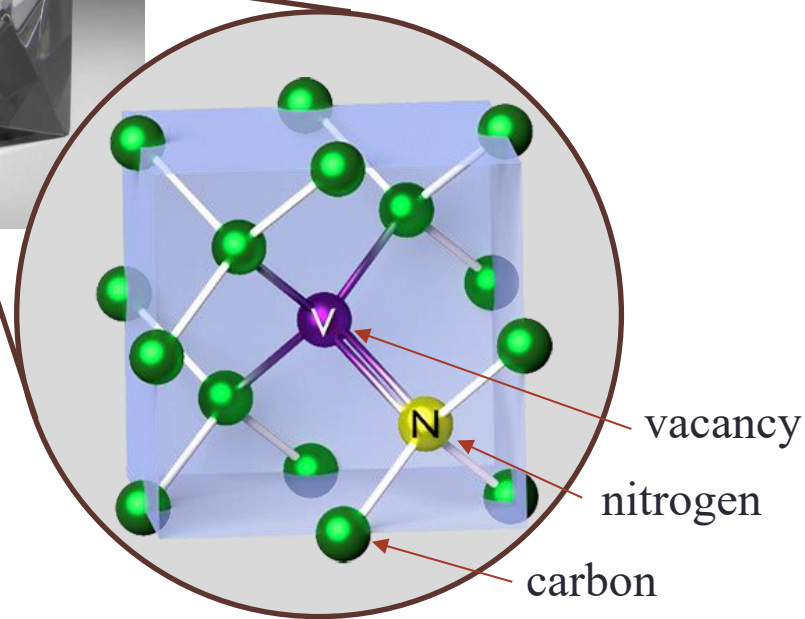
# What is this?

The **NV center** is the first prototypical example of point defect qubits in semiconductors



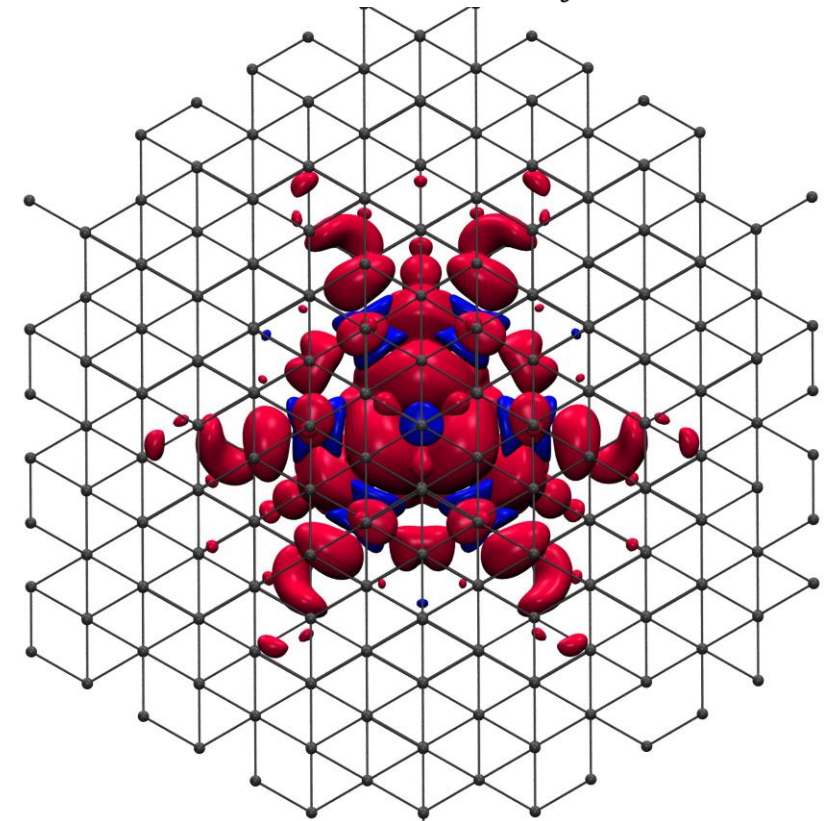
NV center: negatively charged nitrogen substitutional-carbon vacancy complex

Qubit: spin of the NV center



Spin density

$$\rho_{\text{spin}}(\mathbf{r}) = \sum_i^{N_{\text{up}}} |\psi_i^{(\text{up})}(\mathbf{r})|^2 - \sum_j^{N_{\text{down}}} |\psi_j^{(\text{down})}(\mathbf{r})|^2$$



# How to create NV centers?

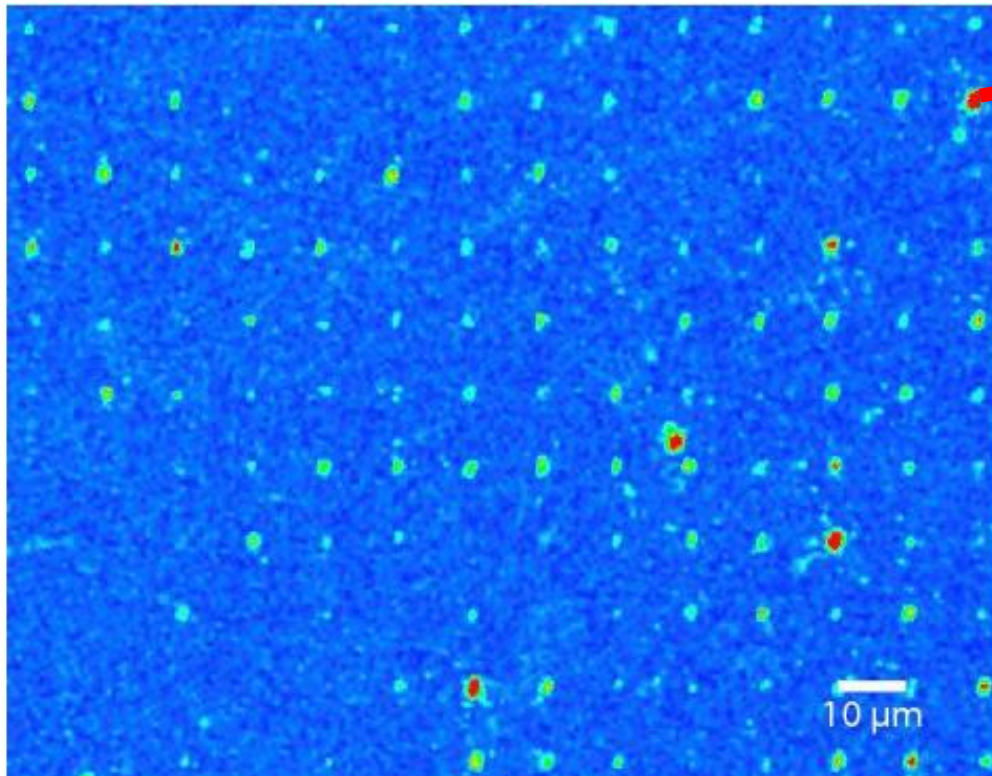
Look for pink natural pink diamonds.

**They may contain  
100 000 000 000 000 000  
NV centers.**

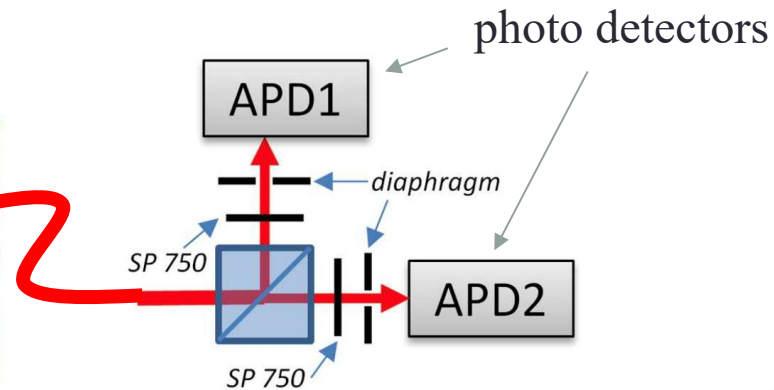


# Controlled fabrication

Nitrogen implanted diamond

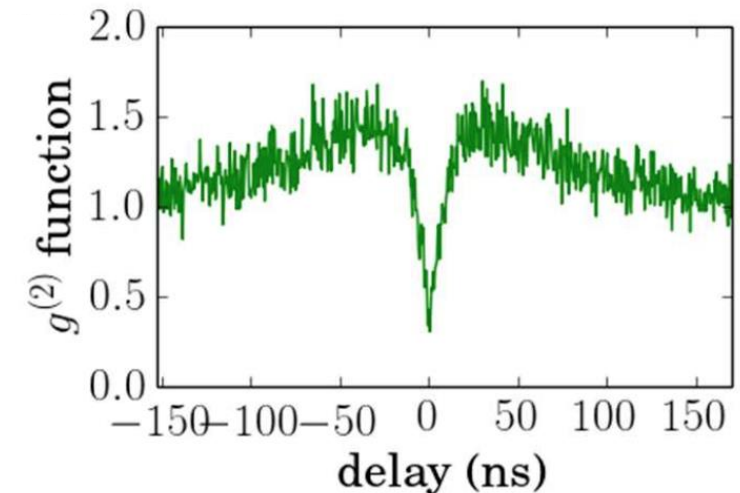


False color image



On demand  
creation of **single**  
NV centers

$$g^{(2)}(\tau) = \frac{\langle : I(t + \tau) I(t) : \rangle}{(\langle I(t) \rangle)^2}$$



Phys. Rev. B **91**, 035308 (2015)

# Quantum Computers - companies

Source:



|          | Electron spins  |         |            | Atoms       |               |  |
|----------|-----------------|---------|------------|-------------|---------------|--|
|          | Superconducting | Silicon | NV Centers | Trapped Ion | Neutral Atoms |  |
| Americas |                 |         |            |             |               |  |
| EMEA     |                 |         |            |             |               |  |
| APAC     |                 |         |            |             |               |  |

Today

 Day (after)<sup>n</sup>  
tomorrow

Tomorrow

# PART II.

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Theory of the NV center

# Basics of group theory

What define your systems are the **structure + number of electrons**  $\longrightarrow$  Symmetry is not everything but effects everything.

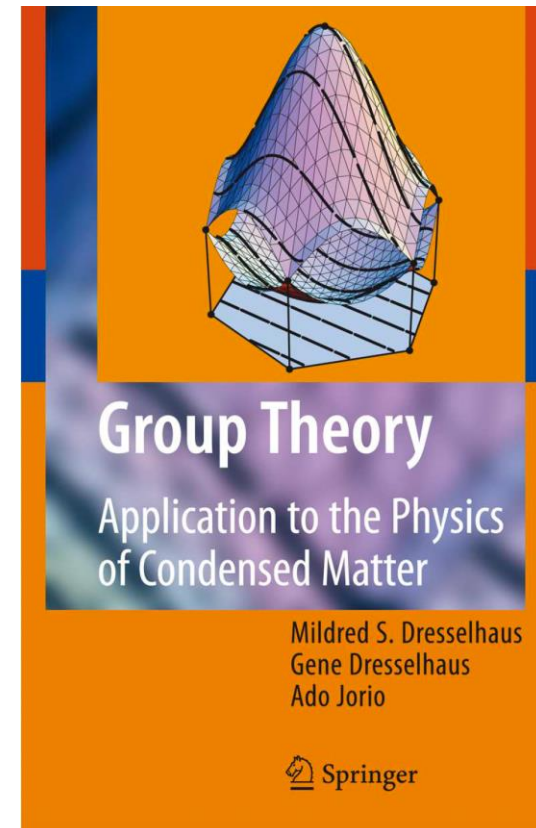
$\uparrow$  has a symmetry

## 1.1 Definition of a Group

A collection of elements  $A, B, C, \dots$  form a group when the following four conditions are satisfied:

1. The product of any two elements of the group is itself an element of the group. For example, relations of the type  $AB = C$  are valid for all members of the group.
2. The associative law is valid – i.e.,  $(AB)C = A(BC)$ .
3. There exists a unit element  $E$  (also called the identity element) such that the product of  $E$  with any group element leaves that element unchanged  $AE = EA = A$ .
4. For every element  $A$  there exists an inverse element  $A^{-1}$  such that  $A^{-1}A = AA^{-1} = E$ .

Page 3 in



# Point groups

Symmetry operations of a structure form a group

- Group elements: symmetry operations
- Product: carry out symmetry operations in sequence

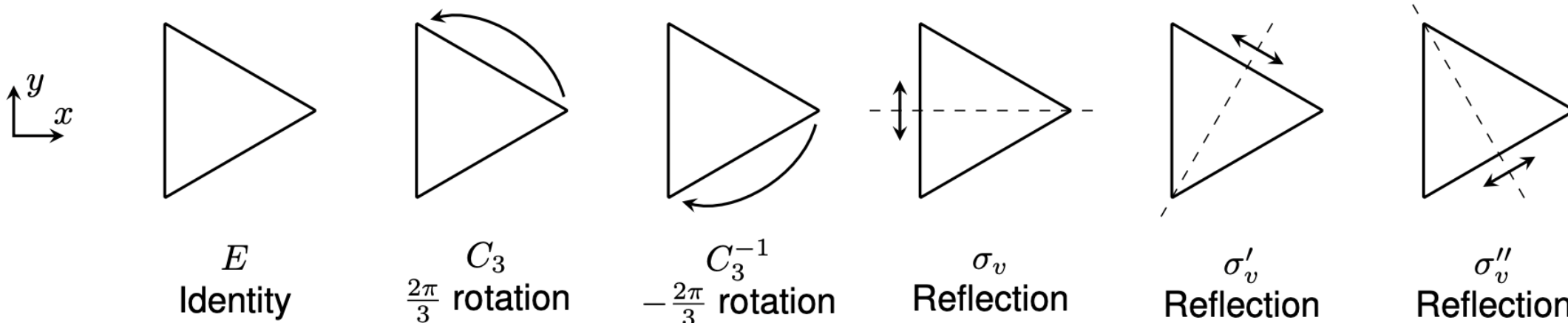
Multiplication table

|              | $E$          | $C_3^+$      | $C_3^-$      | $\sigma_v$   | $\sigma_v'$  | $\sigma_v''$ |
|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| $E$          | $E$          | $C_3^+$      | $C_3^-$      | $\sigma_v$   | $\sigma_v'$  | $\sigma_v''$ |
| $C_3^+$      | $C_3^+$      | $C_3^-$      | $E$          | $\sigma_v''$ | $\sigma_v$   | $\sigma_v'$  |
| $C_3^-$      | $C_3^-$      | $E$          | $C_3^+$      | $\sigma_v'$  | $\sigma_v''$ | $\sigma_v$   |
| $\sigma_v$   | $\sigma_v$   | $\sigma_v'$  | $\sigma_v''$ | $E$          | $C_3^+$      | $C_3^-$      |
| $\sigma_v'$  | $\sigma_v'$  | $\sigma_v''$ | $\sigma_v$   | $C_3^-$      | $E$          | $C_3^+$      |
| $\sigma_v''$ | $\sigma_v''$ | $\sigma_v$   | $\sigma_v'$  | $C_3^+$      | $C_3^-$      | $E$          |

Point groups: all symmetry operations of point groups leave one point of space intact

- No translation symmetry, relevant for polygons, molecules, and **point defects**

Example: Triangle



# Relevnt point groups



## Point Group Symmetry Character Tables

[Chemistry tools](#)[Gas laws](#)[Unit converters](#)[Periodic table](#)[Chemical forum](#)[Constants](#)[Symmetry](#)[Contribute](#)[Contact us](#)**Choose language**[Deutsch](#)[English](#)[Español](#)[Français](#)[Italiano](#)[Nederlands](#) $C_1$  $C_s$  $C_i$  $C_2$  $C_3$  $C_4$  $C_5$  $C_6$  $C_{2v}$  $C_{3v}$  $C_{4v}$  $C_{5v}$  $C_{6v}$  $C_{2h}$  $C_{3h}$  $C_{4h}$  $C_{5h}$  $C_{6h}$  $D_2$  $D_3$  $D_4$  $D_5$  $D_6$  $D_{2h}$  $D_{3h}$  $D_{4h}$  $D_{5h}$  $D_{6h}$  $D_{2d}$  $D_{3d}$  $D_{4d}$  $D_{5d}$  $D_{6d}$  $S_4$  $S_6$  $S_8$  $S_{10}$  $T_d$  $O_h$  $I_h$  $C_{\infty v}$  $D_{\infty h}$

# Representation

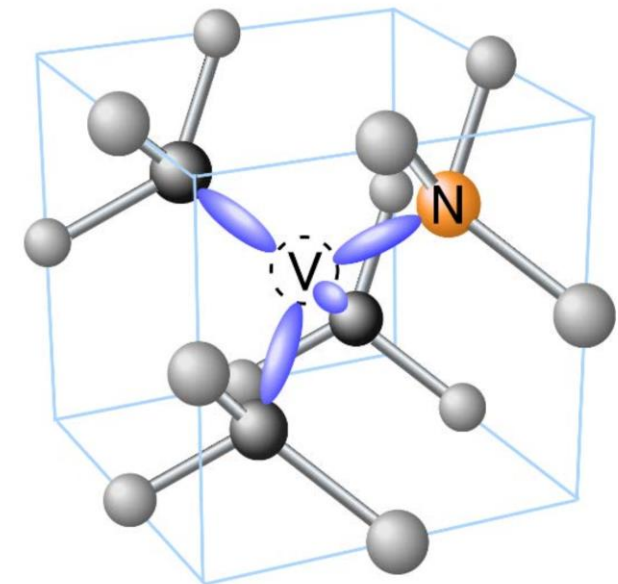
- Representations: Matrix forms (representations) of symmetry operators defined on a vector space that also form a group (isomorphic).

- Elements: square matrices such that  $D(\overset{\text{Symmetry operation}}{\downarrow} A)$
- Product: matrix product such that  $D(AB) = D(A)\overset{\text{Matrix product}}{\downarrow} D(B)$

- Structure:  $3 \times N$  dimensional vector:

$$\mathbf{R} = \{x_1, y_1, z_1, x_2, y_2, z_2, \dots, x_N, y_N, z_N\}$$

$$D(A)\mathbf{R} = \mathbf{R}$$



# Reducible representation

- Matrices of representations are usually sparse matrices.
  - GT says: They can be block diagonalized, i.e. **they are reducible**.

$$D(A) = \begin{pmatrix} 1.0 & 0 & 5.0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3.0 & 0 & 0 & 0 & 0 & 11.0 & 0 \\ 0 & 0 & 0 & 0 & 9.0 & 0 & 0 & 0 \\ 0 & 0 & 6.0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 7.0 & 0 & 0 & 0 & 0 \\ 2.0 & 0 & 0 & 0 & 0 & 10.0 & 0 & 0 \\ 0 & 0 & 0 & 8.0 & 0 & 0 & 0 & 0 \\ 0 & 4.0 & 0 & 0 & 0 & 0 & 0 & 12.0 \end{pmatrix} \xrightarrow{U D(A) U^{-1}} \left( \begin{array}{c|c|c} \Gamma_1 & 0 & \mathcal{O} \\ \hline 0 & \Gamma_1' & \mathcal{O} \\ \hline \mathcal{O} & \mathcal{O} & \Gamma_2 \end{array} \right)$$

3N problem  $\Rightarrow K \times$  smaller problems

# Irreducible representations

$$\left( \begin{array}{c|c|c} \Gamma_1 & 0 & \mathcal{O} \\ \hline 0 & \Gamma_{1'} & \mathcal{O} \\ \hline \mathcal{O} & \mathcal{O} & \Gamma_2 \end{array} \right)$$

Irreducible representations

Reducible and irreducible representations can be characterized by the trace of the matrices, i.e., by their characters

$$\chi^{(\Gamma_j)}(R) = \text{trace } D^{(\Gamma_j)}(R)$$

Character table of the point group symmetry of the triangle

| $\mathbf{C_{3v}}$<br>$h=6$ | $\mathbf{E}$ | $\mathbf{2\ C_3}$ | $\mathbf{3\ \sigma_v}$ |
|----------------------------|--------------|-------------------|------------------------|
| $\mathbf{A_1}$             | 1            | 1                 | 1                      |
| $\mathbf{A_2}$             | 1            | 1                 | -1                     |
| $\mathbf{E}$               | 2            | -1                | 0                      |

# Group theory and quantum mechanics

Structure  $\mathbf{R} \Rightarrow$  Potential  $V(\mathbf{r}) \Rightarrow$  Hamiltonian  $H$

↑ Inherit the symmetry of the structure

$$\mathcal{H}\psi_n = E_n\psi_n$$

$$\hat{P}_R \mathcal{H}\psi_n = \hat{P}_R E_n \psi_n = \mathcal{H}(\hat{P}_R \psi_n) = E_n (\hat{P}_R \psi_n)$$

↑ Exists a group of operators that leave the Hamiltonian unchanged  $[\mathcal{H}, \hat{P}_R] = 0$

↑ Reducible / block diagonalizable matrix

$$\underbrace{\psi'_{n1}, \psi'_{n2}, \dots, \psi'_{ns}}_{\substack{\text{subset 1} \\ \epsilon_1, \Gamma_1}} \underbrace{\psi'_{n,s+1}, \dots, \psi'_{nk}}_{\substack{\text{subset 2} \\ \epsilon_2, \Gamma_2}},$$

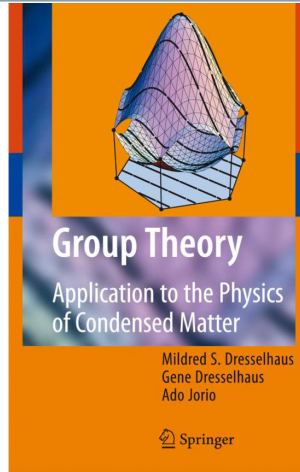
Degenerate subspaces that can be labelled by irreducible representations.

Within a degenerate subset:

$$\hat{P}_R \psi_{n\alpha} = \sum_j D^{(n)}(R)_{j\alpha} \psi_{nj}$$

↑

Irreducible representation of G

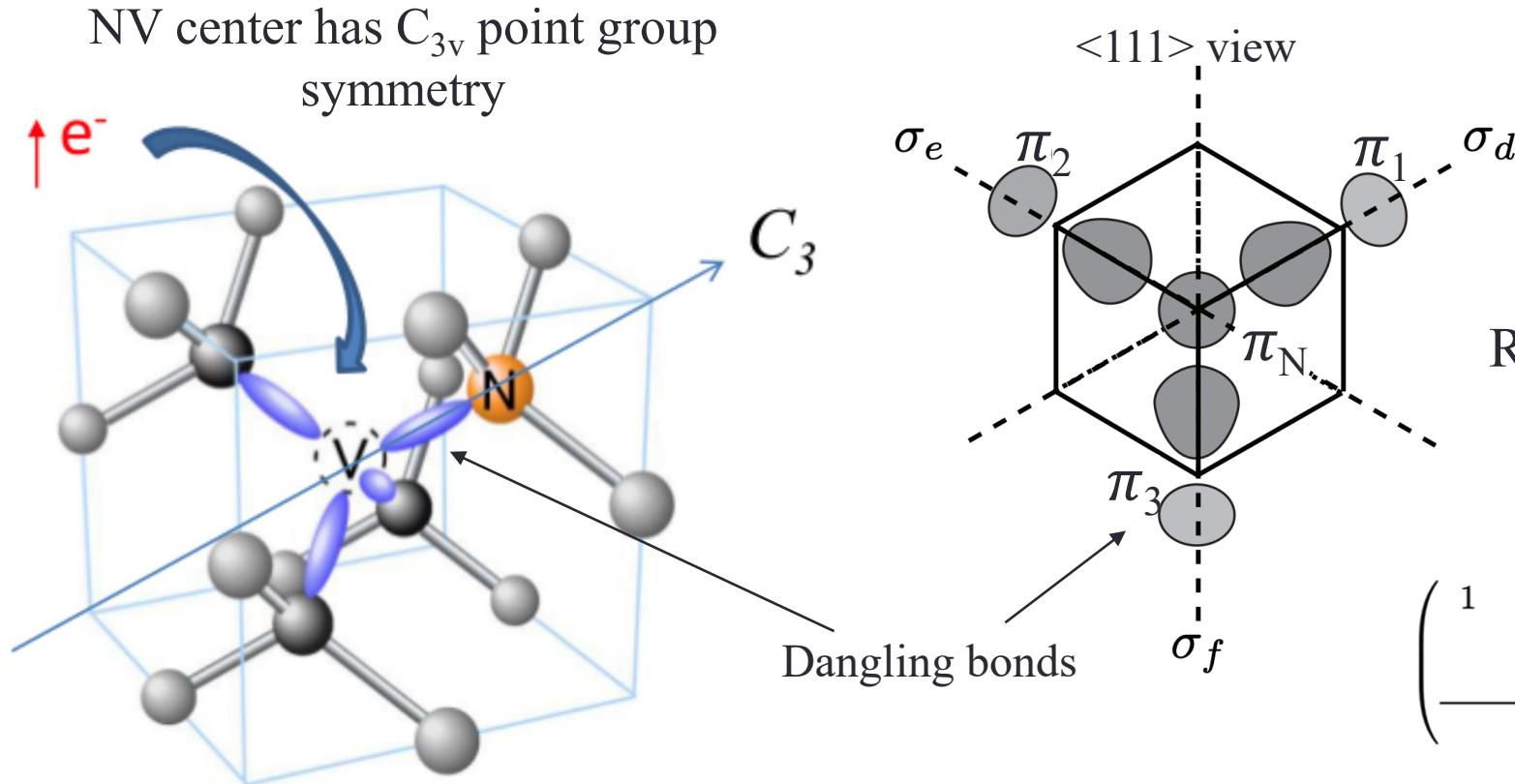


# Splitting of spherical symmetric orbitals in $C_{3v}$ symmetric potential

## Symmetry of Spherical Harmonics (multipoles)

| Angular momentum       | Multipole order         | Symmetry                        | permanent moment? |
|------------------------|-------------------------|---------------------------------|-------------------|
| <b>S</b> ( $\ell=0$ )  | 1 (monopole)            | $A_1$                           |                   |
| <b>P</b> ( $\ell=1$ )  | 2 (dipole)              | $A_1 \oplus E$                  | yes ▼             |
| <b>D</b> ( $\ell=2$ )  | 4 (quadrupole)          | $A_1 \oplus 2 E$                | yes ▼             |
| <b>F</b> ( $\ell=3$ )  | 8 (octupole)            | $2 A_1 \oplus A_2 \oplus 2 E$   | yes ▼             |
| <b>G</b> ( $\ell=4$ )  | 16 (hexadecapole)       | $2 A_1 \oplus A_2 \oplus 3 E$   | yes ▼             |
| <b>H</b> ( $\ell=5$ )  | 32 (dotriacontapole)    | $2 A_1 \oplus A_2 \oplus 4 E$   | yes ▼             |
| <b>I</b> ( $\ell=6$ )  | 64 (tetrahexacontapole) | $3 A_1 \oplus 2 A_2 \oplus 4 E$ | yes ▼             |
| <b>J</b> ( $\ell=7$ )  | 128 (octacosahectapole) | $3 A_1 \oplus 2 A_2 \oplus 5 E$ | yes ▼             |
| <b>K</b> ( $\ell=8$ )  | 256                     | $3 A_1 \oplus 2 A_2 \oplus 6 E$ | yes ▼             |
| <b>L</b> ( $\ell=9$ )  | 512                     | $4 A_1 \oplus 3 A_2 \oplus 6 E$ | yes ▼             |
| <b>M</b> ( $\ell=10$ ) | 1024                    | $4 A_1 \oplus 3 A_2 \oplus 7 E$ | yes ▼             |

# Application to the NV center



Reducible representation  $\hat{P}_R$  defined on the basis of  $\pi_1$ ,  $\pi_2$ ,  $\pi_3$ , and  $\pi_N$

$$\begin{array}{ccc}
 E & C_3^+ & C_3^- \\
 \left( \begin{array}{cc|c} 1 & & \\ & 1 & \\ \hline & & 1 \end{array} \right) & \left( \begin{array}{cc|c} & & 1 \\ 1 & & \\ \hline & & 1 \end{array} \right) & \left( \begin{array}{cc|c} & & 1 \\ & 1 & \\ \hline 1 & & 1 \end{array} \right) \\
 \sigma_d & \sigma_e & \sigma_f
 \end{array}$$
  

$$\Rightarrow
 \begin{array}{ccc}
 \left( \begin{array}{cc|c} 1 & & \\ & 1 & \\ \hline & & 1 \end{array} \right) & \left( \begin{array}{cc|c} & & 1 \\ 1 & & \\ \hline & & 1 \end{array} \right) & \left( \begin{array}{cc|c} & & 1 \\ & 1 & \\ \hline 1 & & 1 \end{array} \right)
 \end{array}$$

Already partially block diagonal  $\Rightarrow$

# Block diagonalization of the representation

- GT projector operators: provide symmetric basis functions from non-symmetric ones.

$$\hat{P}^{(\Gamma_n)} = \frac{\ell_n}{h} \sum_R \chi^{(\Gamma_n)}(R)^* \hat{P}_R$$

Sum over all symmetry elements  $\rightarrow$   $\sum_R$

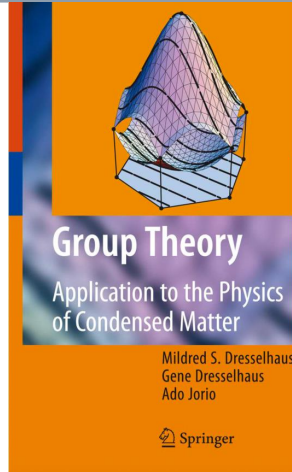
Character of representation  $\Gamma$  of symmetry element  $R$ .  $\rightarrow$   $\chi^{(\Gamma_n)}(R)^*$

Symmetry operator acts on the orbitals  $\rightarrow$   $\hat{P}_R$

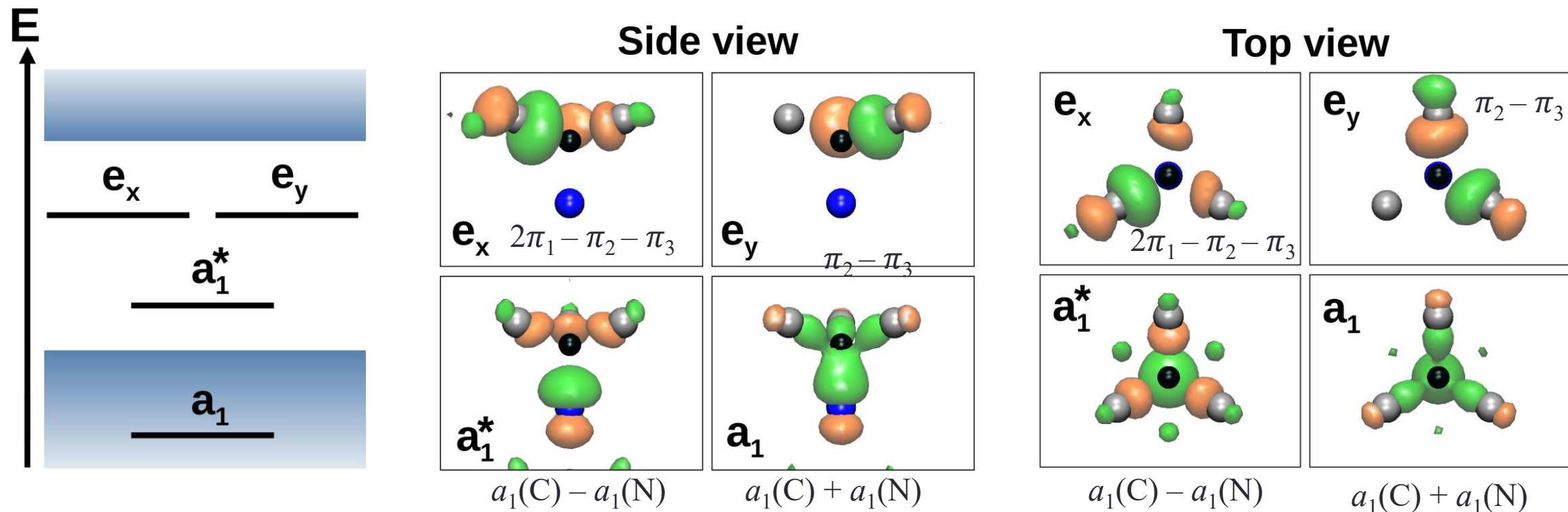
| $\mathbf{C_{3v}}$<br>$h=6$ | <b>E</b> | <b>2 C<sub>3</sub></b> | <b>3 σ<sub>v</sub></b> |
|----------------------------|----------|------------------------|------------------------|
| <b>A<sub>1</sub></b>       | 1        | 1                      | 1                      |
| <b>A<sub>2</sub></b>       | 1        | 1                      | -1                     |
| <b>E</b>                   | 2        | -1                     | 0                      |

Irreducible basis:

- $a_1(\text{N}) = \pi_{\text{N}}$
- $a_1(\text{C}) = (\pi_1 + \pi_2 + \pi_3)/\sqrt{3}$
- $e = \{(2\pi_1 - \pi_2 - \pi_3)/\sqrt{6}, (\pi_2 - \pi_3)/\sqrt{2}\}$



# How does it look in the single-particle DFT method?



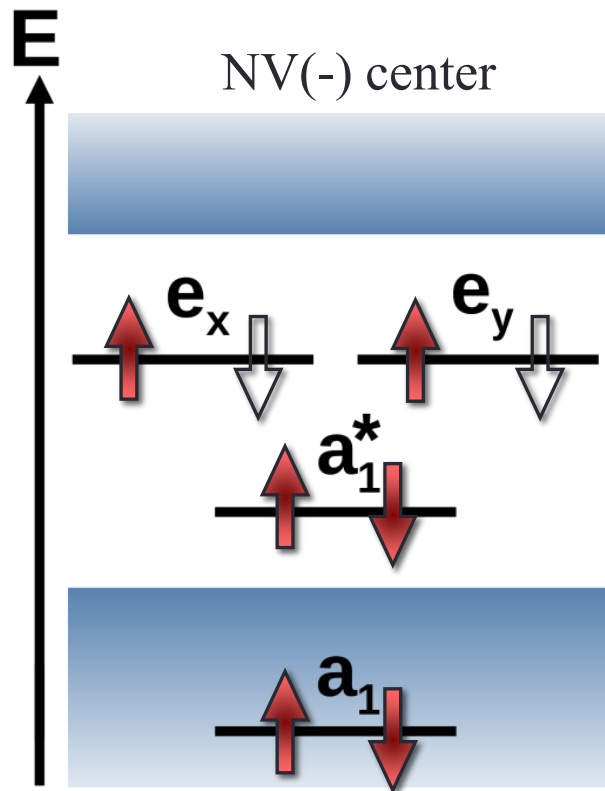
DFT knows group theory!  
 $V(\mathbf{r})$  is symmetric

Group theory does not tell you where  
 these states are in the band structure  
 of diamond.

# Let's occupy the states with electrons

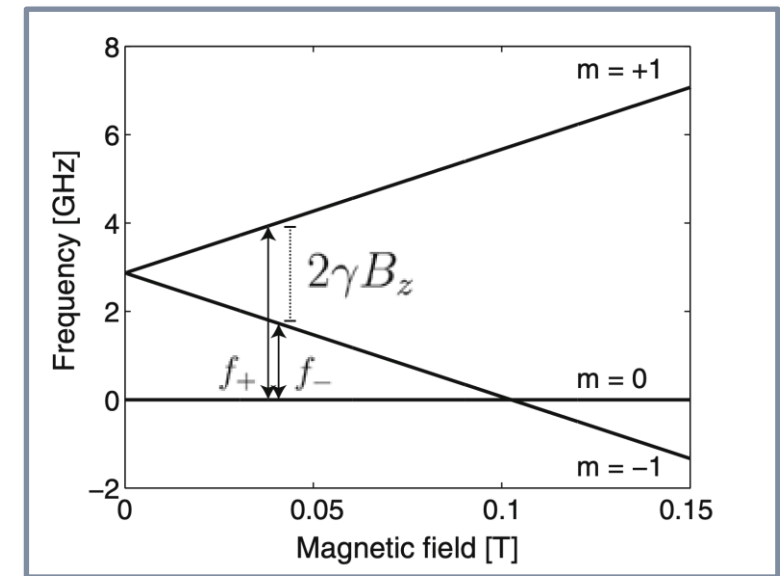
Number of electrons:

2 from N, 3 from 3 carbons, and 1 from the environment = 6



Triplet ground state

$$S = 1; \quad m_S = \{-1, 0, +1\}$$



NV electron spin qubit:

- 2 states of the electron spin can form a qubit
- Coherent control via microwave irradiation
- Tuning with an external magnetic field
- **How can we read out and initialize?**

## We need more group theory!

- Irreducible representation of the possible many-body WFs can be obtained by including all electrons and their spin:

$$\Gamma_{\Psi} = \prod_n (\Gamma_{hn} \otimes D_{1/2})$$

$\uparrow$  Irrep of the electron spin-1/2 in  $C_{3v}$   
 $\uparrow$  Irrep of the spatial part (orbital)

Projectors can be used to obtain the symmetry-allowed states of the many-body system.

$$\Psi^r = P^{(r)} \varphi_1 \otimes \chi_1 \otimes \varphi_2 \otimes \chi_2 = \frac{l_r}{h} \sum_e \chi_e^{(r)*} R_e \varphi_1 \otimes U_e \chi_1 \otimes R_e \varphi_2 \otimes U_e \chi_2$$

# Many-body spe

 ${}^3E$ 

$$\begin{aligned} A_1 &= |E_-\rangle \otimes |\alpha\alpha\rangle - |E_+\rangle \otimes |\beta\beta\rangle \\ A_2 &= |E_-\rangle \otimes |\alpha\alpha\rangle + |E_+\rangle \otimes |\beta\beta\rangle \\ E_1 &= |E_-\rangle \otimes |\beta\beta\rangle - |E_+\rangle \otimes |\alpha\alpha\rangle \\ E_2 &= |E_-\rangle \otimes |\beta\beta\rangle + |E_+\rangle \otimes |\alpha\alpha\rangle \\ E_y &= |Y\rangle \otimes |\alpha\beta + \beta\alpha\rangle \\ E_x &= |X\rangle \otimes |\alpha\beta + \beta\alpha\rangle \end{aligned}$$

$$\begin{aligned} {}^3A_{2-} &= \\ {}^3A_{20} &= |e_x e_y - e_y e_x\rangle \otimes \begin{cases} |\beta\beta\rangle \\ |\alpha\beta + |\beta\alpha\rangle \\ \alpha\alpha\rangle \end{cases} \\ {}^3A_{2+} &= \end{aligned}$$

| Triplet states<br>(S=1)                                                                                                                          | Energy $E$ |  | Singlet states<br>(S=0)                                                                                                                                                                                                                                                                                          |                                              |                          |
|--------------------------------------------------------------------------------------------------------------------------------------------------|------------|--|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------|--------------------------|
|                                                                                                                                                  |            |  | $\uparrow\uparrow\uparrow$<br>$\uparrow\uparrow$<br>$-$<br>${}^1A_1'''$                                                                                                                                                                                                                                          | $a_1 \rightarrow e$<br>$a_1 \rightarrow e$   | 2nd order<br>excitations |
| $\uparrow\uparrow\uparrow$<br>$\uparrow$<br>$\uparrow$<br>${}^3A_1$                                                                              |            |  | $\uparrow\uparrow\uparrow$ $\uparrow\uparrow\uparrow$<br>$\uparrow$ $-$ $\uparrow$<br>$\uparrow$ $\uparrow$<br>${}^1A_1''$                                                                                                                                                                                       | $a_1' \rightarrow e$<br>$a_1 \rightarrow e$  |                          |
| Expected<br>additional states                                                                                                                    |            |  | $\uparrow\uparrow\uparrow$<br>$-$<br>$\uparrow\uparrow$<br>${}^1A_1'$                                                                                                                                                                                                                                            | $a_1' \rightarrow e$<br>$a_1' \rightarrow e$ |                          |
| $\uparrow\uparrow\uparrow$ $\uparrow\uparrow\uparrow$<br>$\uparrow\uparrow$ $\uparrow\uparrow$<br>$\uparrow$ $\uparrow$<br>${}^3E'_x$ ${}^3E'_y$ |            |  | $\uparrow\uparrow\uparrow$ $\uparrow\uparrow\uparrow$ $\uparrow\uparrow\uparrow$ $\uparrow\uparrow\uparrow$<br>$\uparrow\uparrow$ $-$ $\uparrow\uparrow$ $\uparrow\uparrow$ $-$ $\uparrow\uparrow$<br>$\uparrow$ $\uparrow$ $\uparrow$ $\uparrow$ $\uparrow$ $\uparrow$<br>${}^1E''_x$ ${}^1E''_y$               | $a_1 \rightarrow e$                          | 1st order<br>excitations |
| $\uparrow\uparrow\uparrow$ $\uparrow\uparrow\uparrow$<br>$\uparrow$ $\uparrow$<br>$\uparrow\uparrow$ $\uparrow\uparrow$<br>${}^3E_x$ ${}^3E_y$   |            |  | $\uparrow\uparrow\uparrow$ $\uparrow\uparrow\uparrow$ $\uparrow\uparrow\uparrow$ $\uparrow\uparrow\uparrow$<br>$\uparrow$ $-$ $\uparrow$ $\uparrow$ $-$ $\uparrow$<br>$\uparrow\uparrow$ $\uparrow\uparrow$ $\uparrow\uparrow$ $\uparrow\uparrow$<br>${}^1E'_x$ ${}^1E'_y$                                       | $a_1' \rightarrow e$                         |                          |
| Spin polarization<br>cycle                                                                                                                       |            |  | $- \uparrow\uparrow \uparrow\uparrow -$<br>$\uparrow\uparrow + \uparrow\uparrow$<br>$\uparrow\uparrow$<br>${}^1A_1$                                                                                                                                                                                              | $e \rightarrow e$                            | 0th order<br>excitations |
| $\uparrow\uparrow$<br>$\uparrow\uparrow$<br>$\uparrow\uparrow$<br>${}^3A_2$                                                                      |            |  | $\uparrow\uparrow$ $\uparrow\uparrow$ $\uparrow\uparrow$ $\uparrow\uparrow$ $- \uparrow\uparrow \uparrow\uparrow -$<br>$\uparrow\uparrow$ $-$ $\uparrow\uparrow$ $\uparrow\uparrow$ $-$ $\uparrow\uparrow$<br>$\uparrow\uparrow$ $\uparrow\uparrow$ $\uparrow\uparrow$ $\uparrow\uparrow$<br>${}^1E_x$ ${}^1E_y$ |                                              |                          |

$$\begin{aligned} {}^1E_1 &= |e_x e_x - e_y e_y\rangle \\ {}^1E_2 &= |e_x e_y + e_y e_x\rangle \\ {}^1A_1 &= |e_x e_x + e_y e_y\rangle \end{aligned} \left. \vphantom{\begin{aligned} {}^1E_1 \\ {}^1E_2 \\ {}^1A_1 \end{aligned}} \right\} \otimes |\alpha\beta - \beta\alpha\rangle$$

# Many-body electronic structure and allowed transitions

## Selection rules

Non-zerosness of matrix elements of the operators can be obtained from group theory.

- Optical transition (red arrows):

$$\mu_{fi} = \langle \Psi_f | e\hat{\mathbf{r}} | \Psi_i \rangle$$

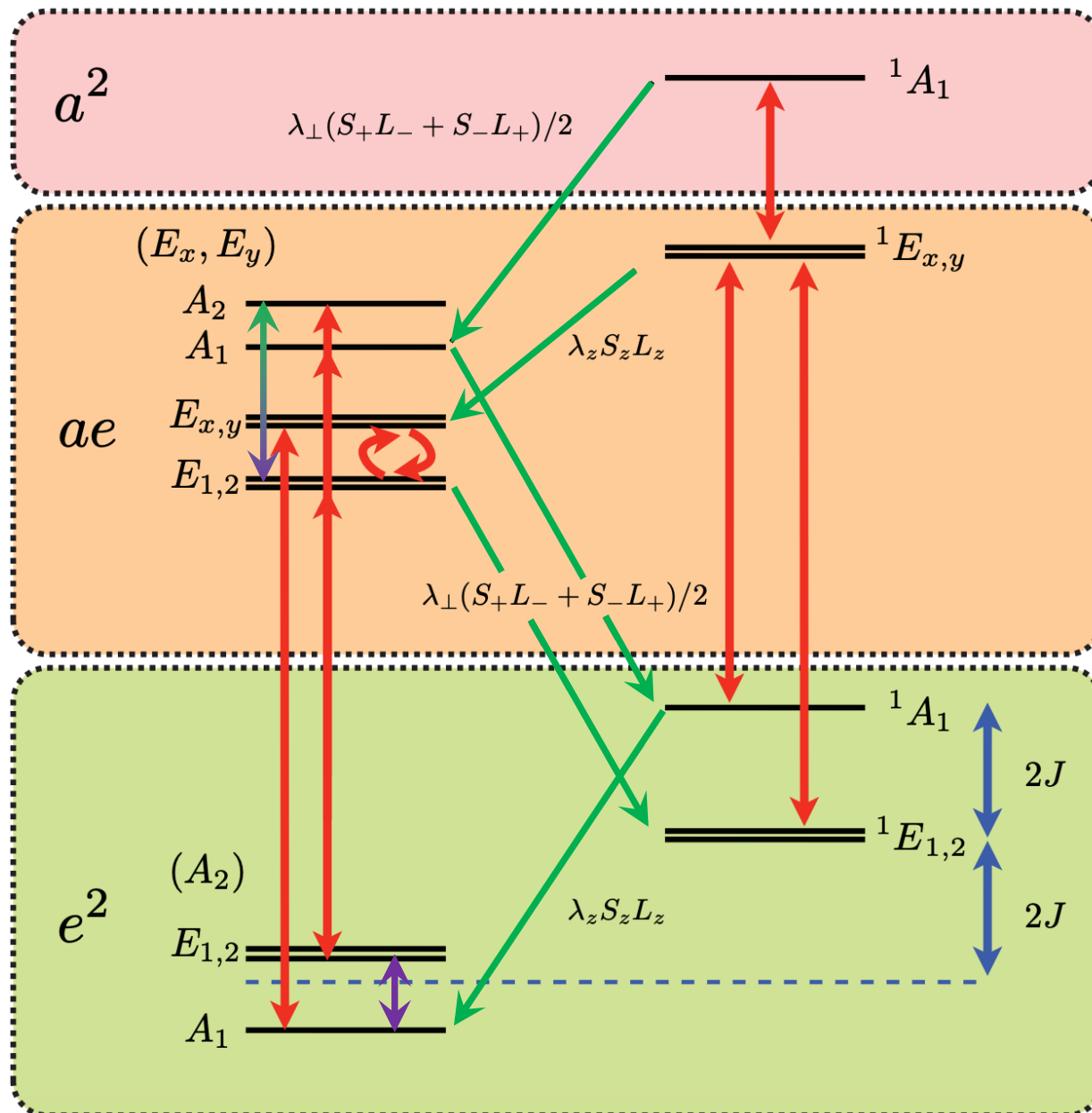
$$\mu_{fi} \neq 0 \quad \text{only if} \quad A_1 \subset \Gamma_f \otimes \Gamma_{\text{er}} \otimes \Gamma_i$$

- Spin-spin interaction (purple arrows):

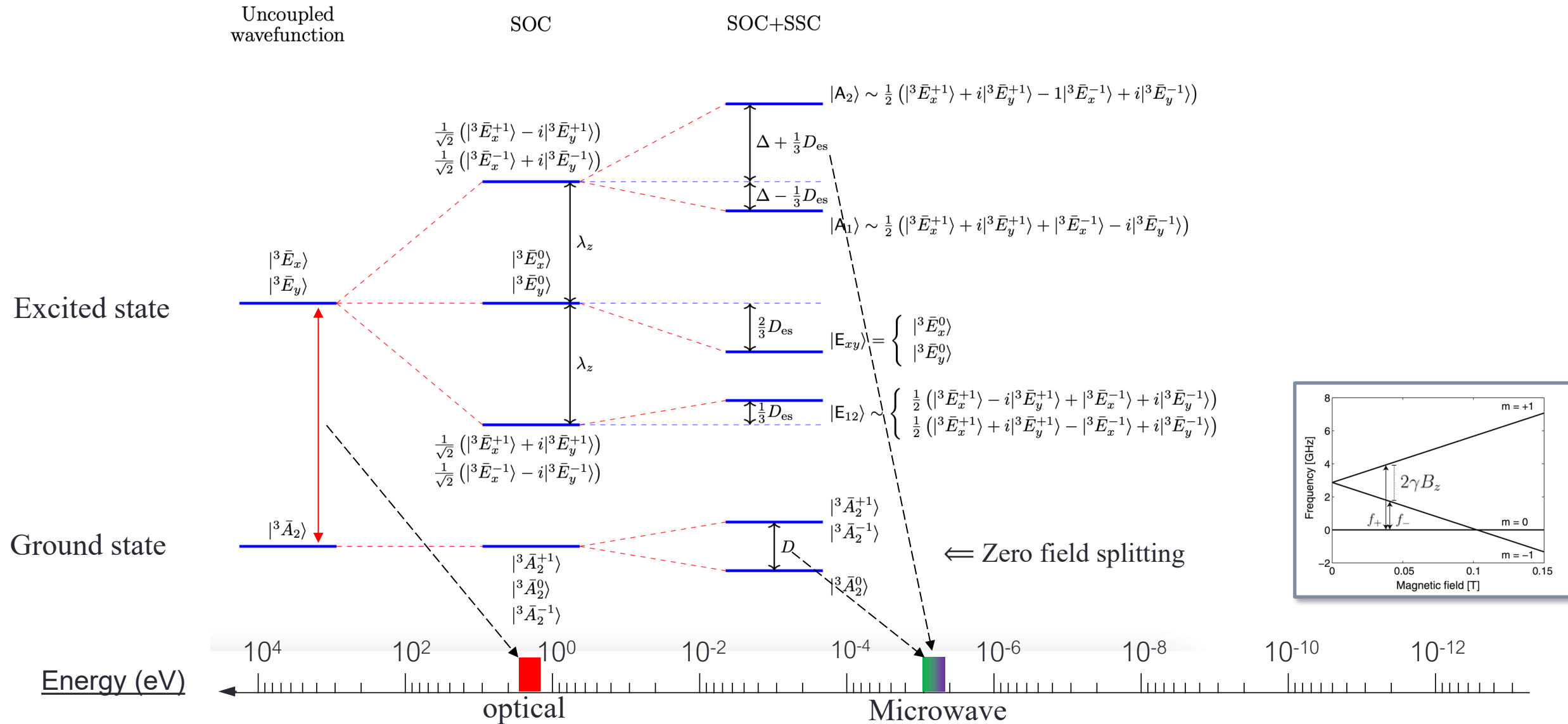
$$h_{ss} = -\frac{\mu_0}{4\pi} \frac{g^2 \beta^2}{r^3} (3(\mathbf{s}_1 \cdot \hat{r})(\mathbf{s}_2 \cdot \hat{r}) - \mathbf{s}_1 \cdot \mathbf{s}_2)$$

- Spin-orbit interaction (green arrows):

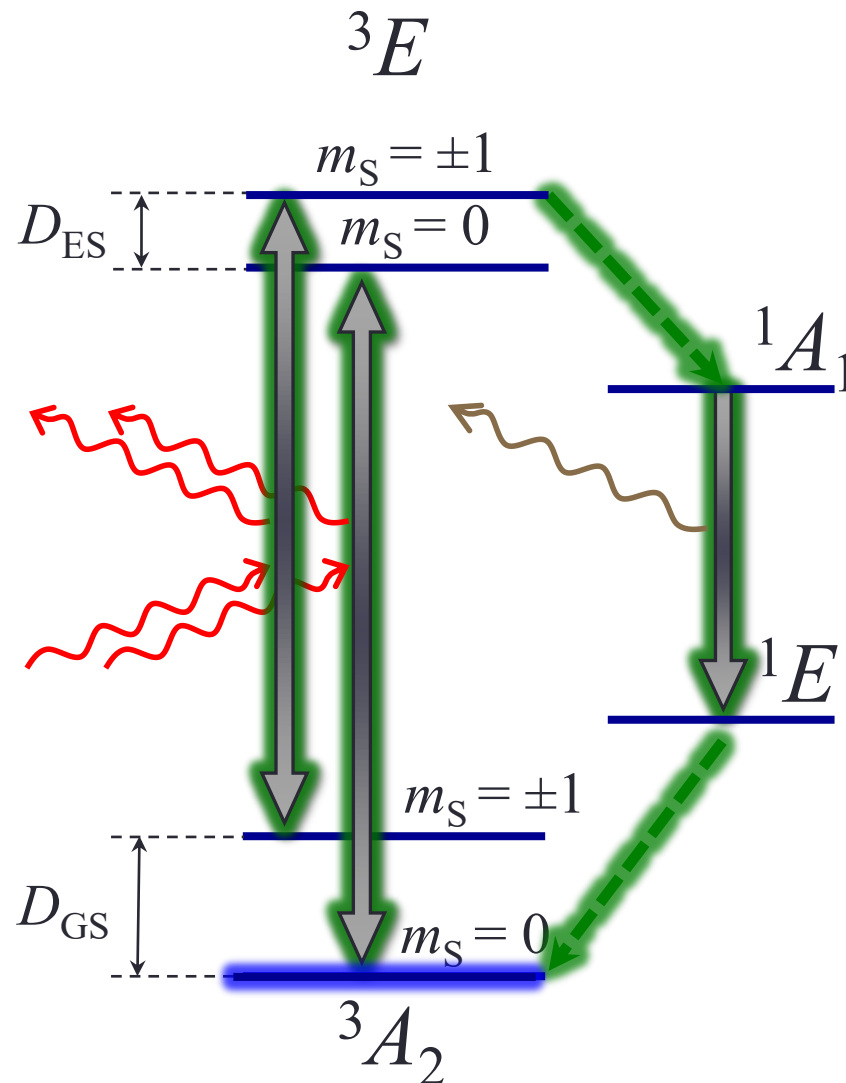
$$H_{SO} = \sum_k \frac{1}{2} \frac{\hbar}{c^2 m_e^2} (\nabla_k V \times \mathbf{p}_k) \cdot \left( \frac{\mathbf{s}_k}{\hbar} \right)$$



# Ground and excited state fine structure



We can now understand how spin initialization and readout work.



**Initilization with optical pumping:**

State is in  $m_S = 0 \Rightarrow$  stays there

State is in  $m_S = \pm 1 \Rightarrow$  stays there  
 $\Rightarrow$  decay to  $m_S = 0$

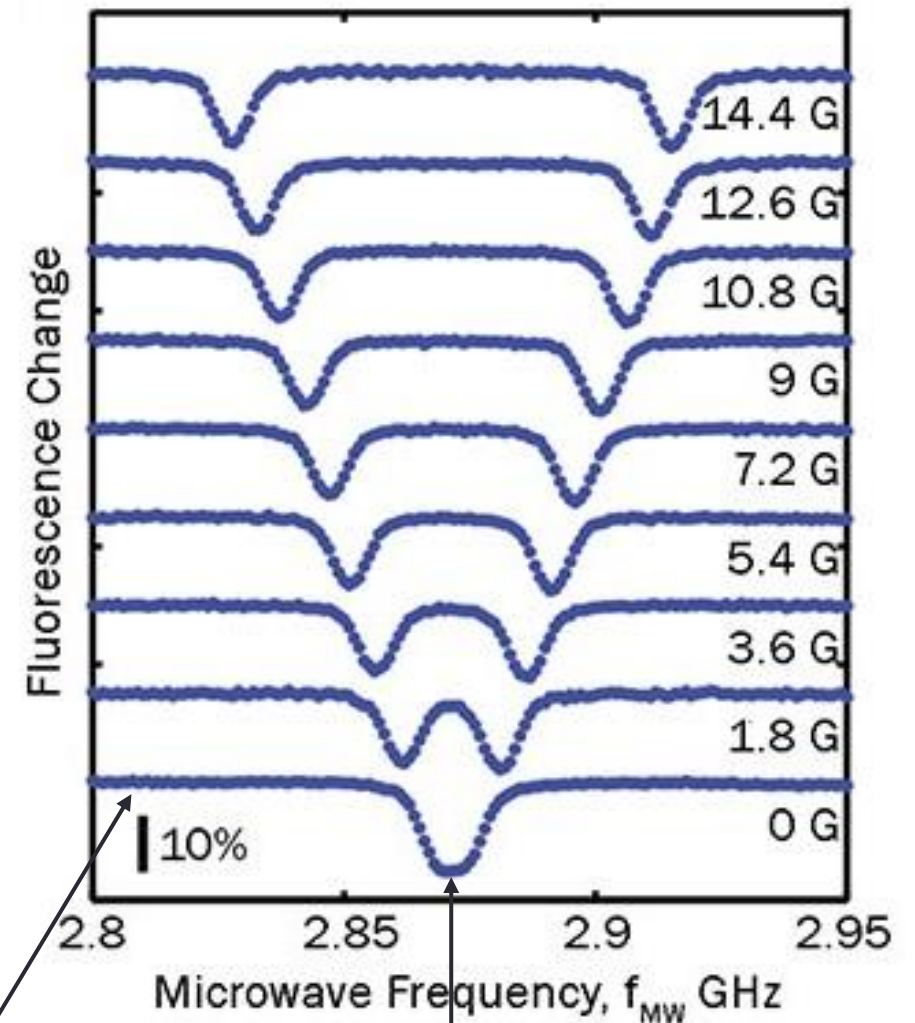
The result of many optical cycling:  
 Initialization with 95% probability  
 in  $m_S = 0$



# Optically detected magnetic resonance

Continuous wave ODMR:

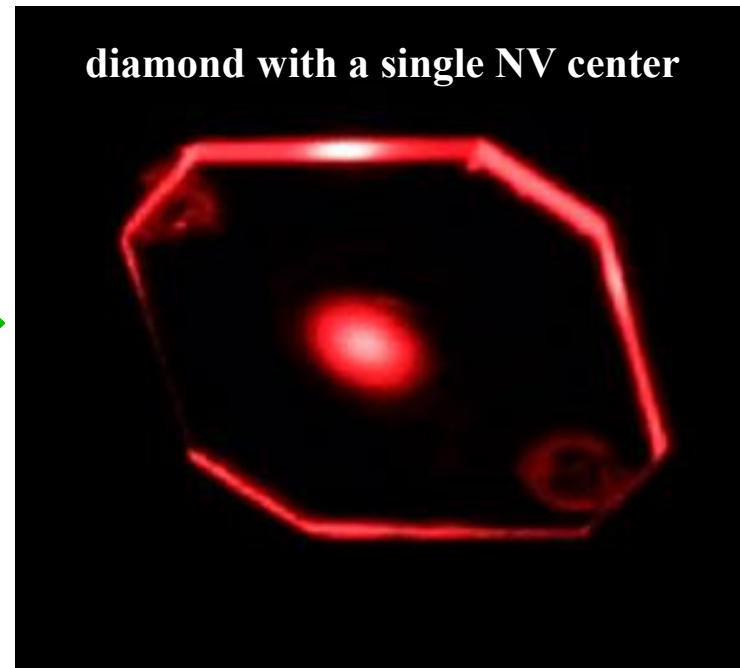
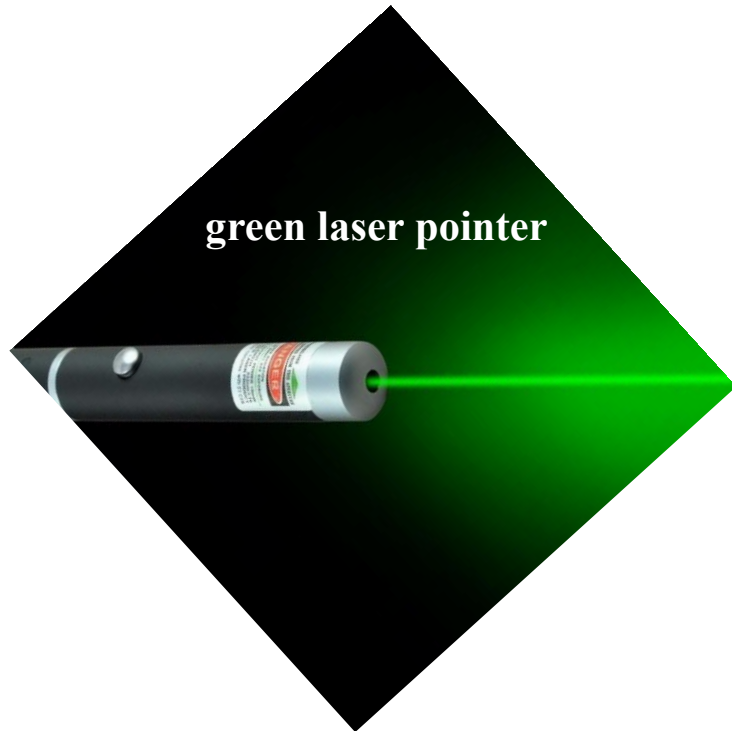
- Apply optical excitation
- Apply MW excitation
- Sweep the MW frequency
- (Sweep the magnetic field)



Off resonant MW:  $m_S = 0$

Resonant MW: 50%  $m_S = 0$  + 50%  $m_S = \pm 1$

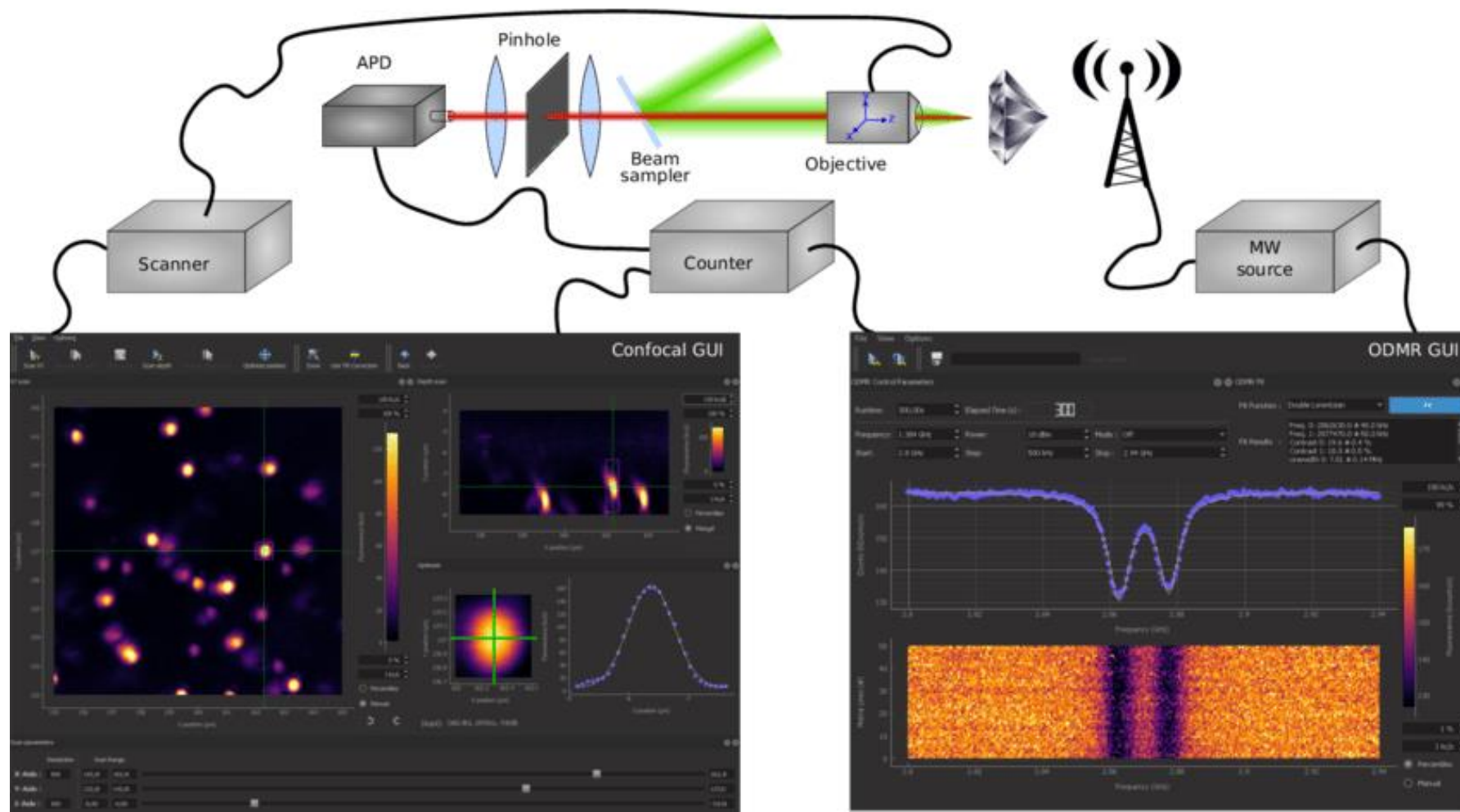
# DIY: room temperature quantum control



microwave source (1-2 GHz)



# More professional way: confocal microscopy setup



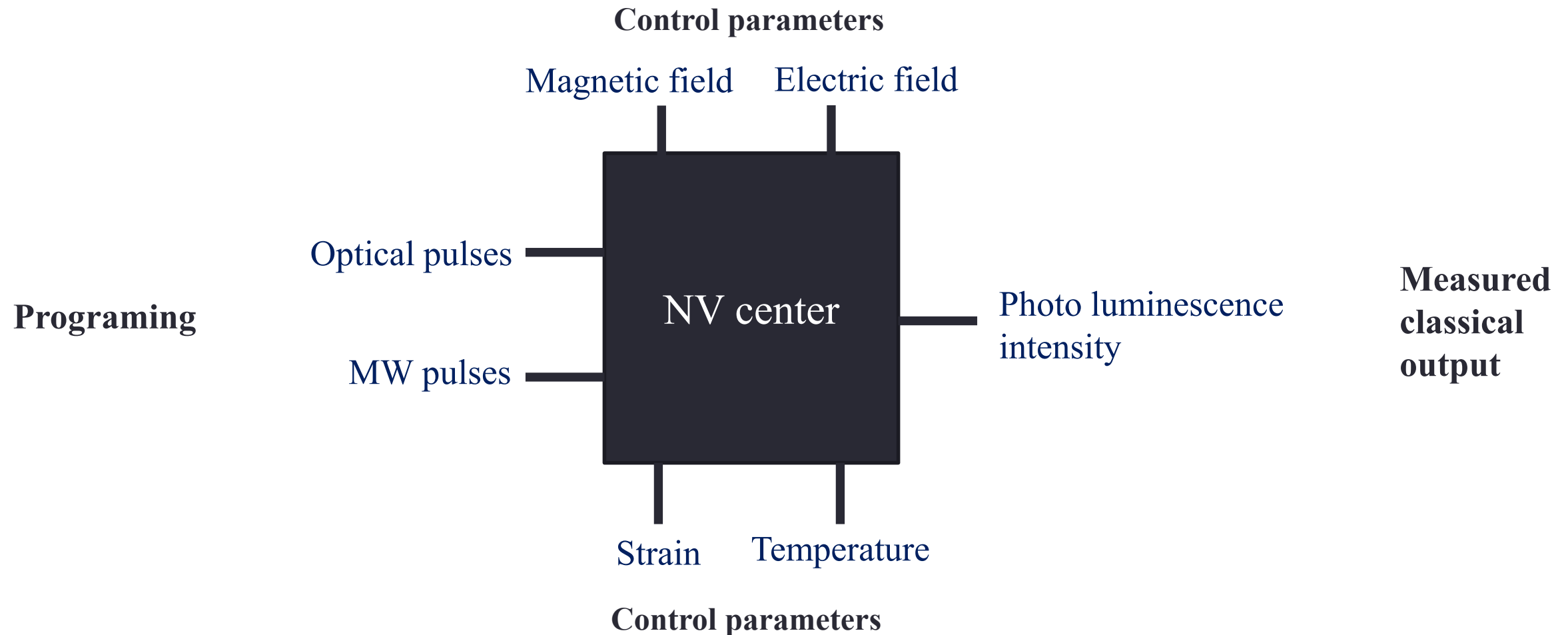
# High temperature spin control?

How is it possible?

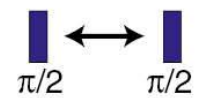
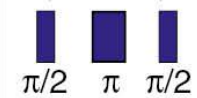
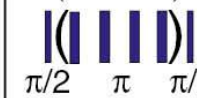
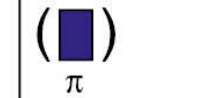
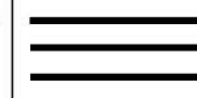
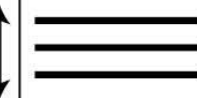
Short answer is: it is quantum mechanics!

- The localized defect states decouple from the bath of diamond electrons.
- Magnetic dipole interaction is much weaker than the electrostatic interaction
- No spin-orbit coupling in the ground state
- Low magnetic noise in diamond samples:
  - Low concentration of electron spins, i.e., high-quality diamond samples available.
  - Low concentration of nuclear spins, 1%  $^{13}\text{C}$  spin-1/2 nuclear spin abundance.
- $\Rightarrow$  spin states are preserved (even at 1400K)
- Read out works: demonstrates the rigour of selection rules.

# Summary of control of the NV center



# Instructions, standard NMR pulse sequences

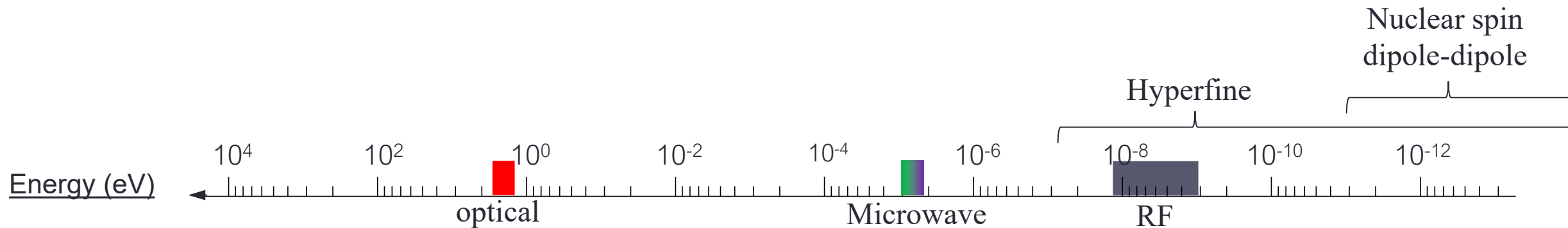
|                 | CW ODMR                                                                             | Pulsed ODMR                                                                                | Ramsey                                                                                                 | Hahn echo                                                                                                    | Dynamical decoupling                                                                                         | Rabi                                                                                         | T1 relaxometry                                                                               |
|-----------------|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------|
| Laser           |    |          |                     |                           |                           |           |           |
| Microwave       |    | <br>$\pi$ | <br>$\pi/2$ $\pi/2$ | <br>$\pi/2$ $\pi$ $\pi/2$ | <br>$\pi/2$ $\pi$ $\pi/2$ | <br>$\pi$ | <br>$\pi$ |
| Readout         |    |          |                     |                           |                           |           |           |
| Bias field      |    |          |                     |                           |                           |          |          |
| Sample field    |  |        |                   |                         |                         |         |         |
| Swept parameter | Microwave frequency                                                                 | Microwave frequency                                                                        | Free precession time, $\tau$                                                                           | Spin evolution time, $\tau$                                                                                  | Spin evolution time, $\tau$                                                                                  | Microwave pulse duration, bias field                                                         | Laser pulse delay, bias field                                                                |

# Interaction with the environment

- Spin Hamiltonian:

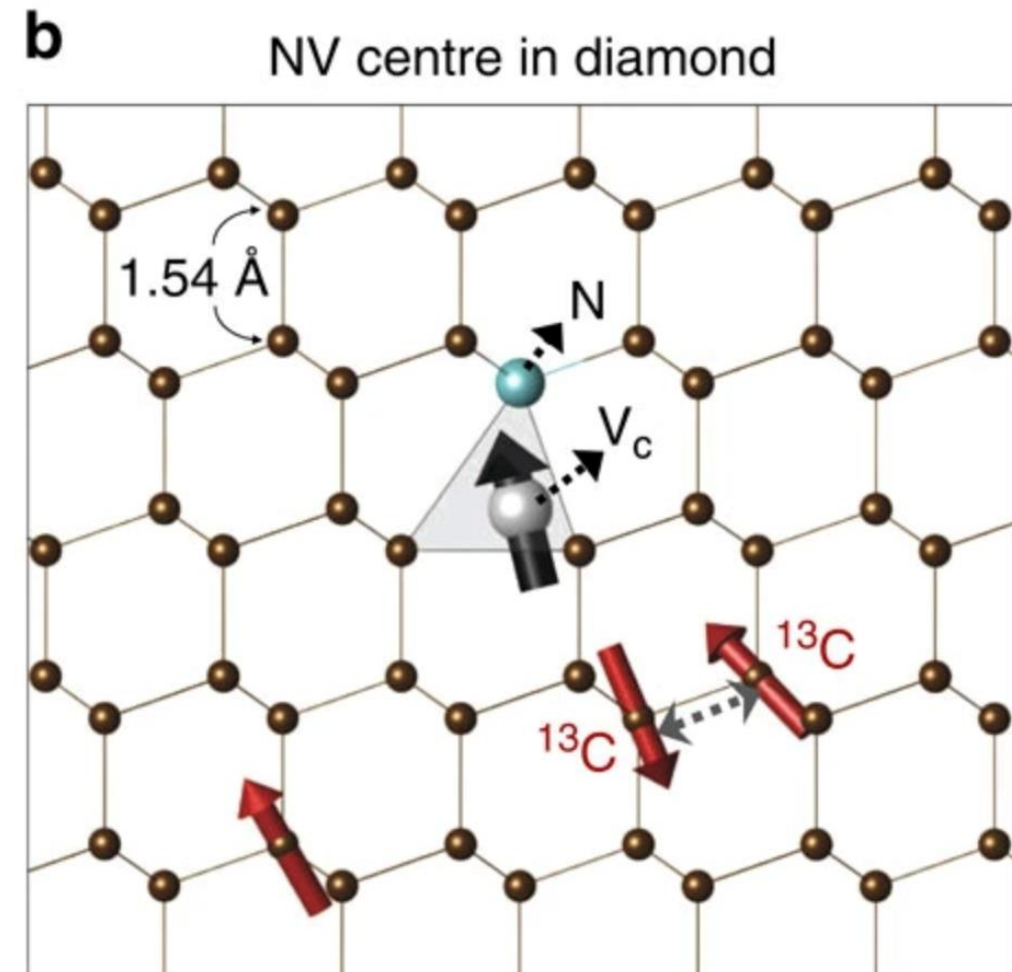
Strain and electric field dependent

$$\hat{H} = \hat{H}_e + \hat{H}_b + \hat{H}_{e-b} = D \left( \hat{S}_z^2 - S(S+1)/3 \right) + \frac{E}{2} \left( \hat{S}_+^2 + \hat{S}_-^2 \right) + g_e \mu_B \mathbf{B}^T \hat{\mathbf{S}} - \sum_i g_N^{(i)} \mu_N^{(i)} \mathbf{B}^T \hat{\mathbf{I}}^{(i)} + \sum_i \hat{\mathbf{I}}^{(i)} \mathbf{Q}^{(i)} \hat{\mathbf{I}}^{(i)} + \sum_{i < j} \hat{\mathbf{I}}^{T(i)} \mathbf{J}^{(ij)} \hat{\mathbf{I}}^{(j)} + \sum_i \hat{\mathbf{S}}^T \mathbf{A}^{(i)} \hat{\mathbf{I}}^{(i)},$$



# Nuclear spins as sources of decoherence

- Dipole-dipole interaction with  $^{13}\text{C}$  nuclear spins is the major source of decoherence,  $\Rightarrow$  spinless  $^{12}\text{C}$  isotope enrichment.
  - Open quantum system (?)
  - Electron spin is surrounded by a bath of quantum memories.
    - Nuclear spin coherence time can exceed seconds at room temperature in diamond
  - The cluster correlation expansion (CCE) method works very well in a parameter-free manner.



# Introduction of the CCE method

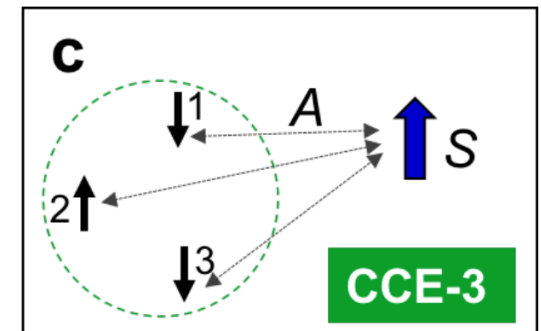
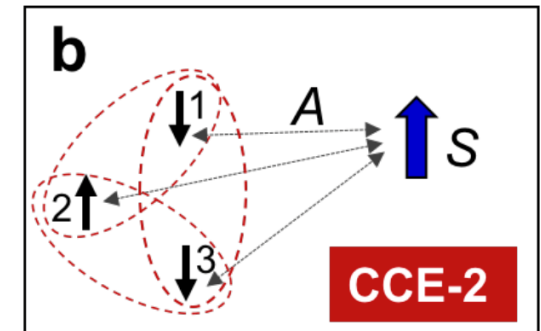
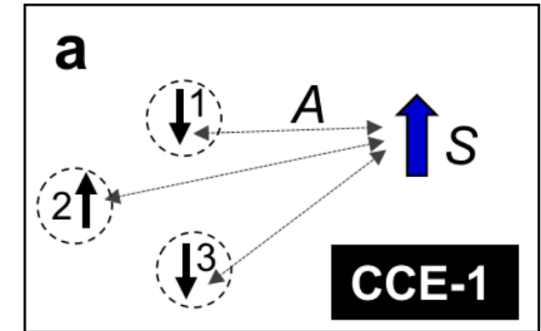
Electron spin's density matrix:  $\varrho_e(t) = \text{Tr}_{\text{bath}} \varrho(t)$

Coherence function:  $L(t) = \text{Tr}(\sigma_+ \varrho_e(t))$

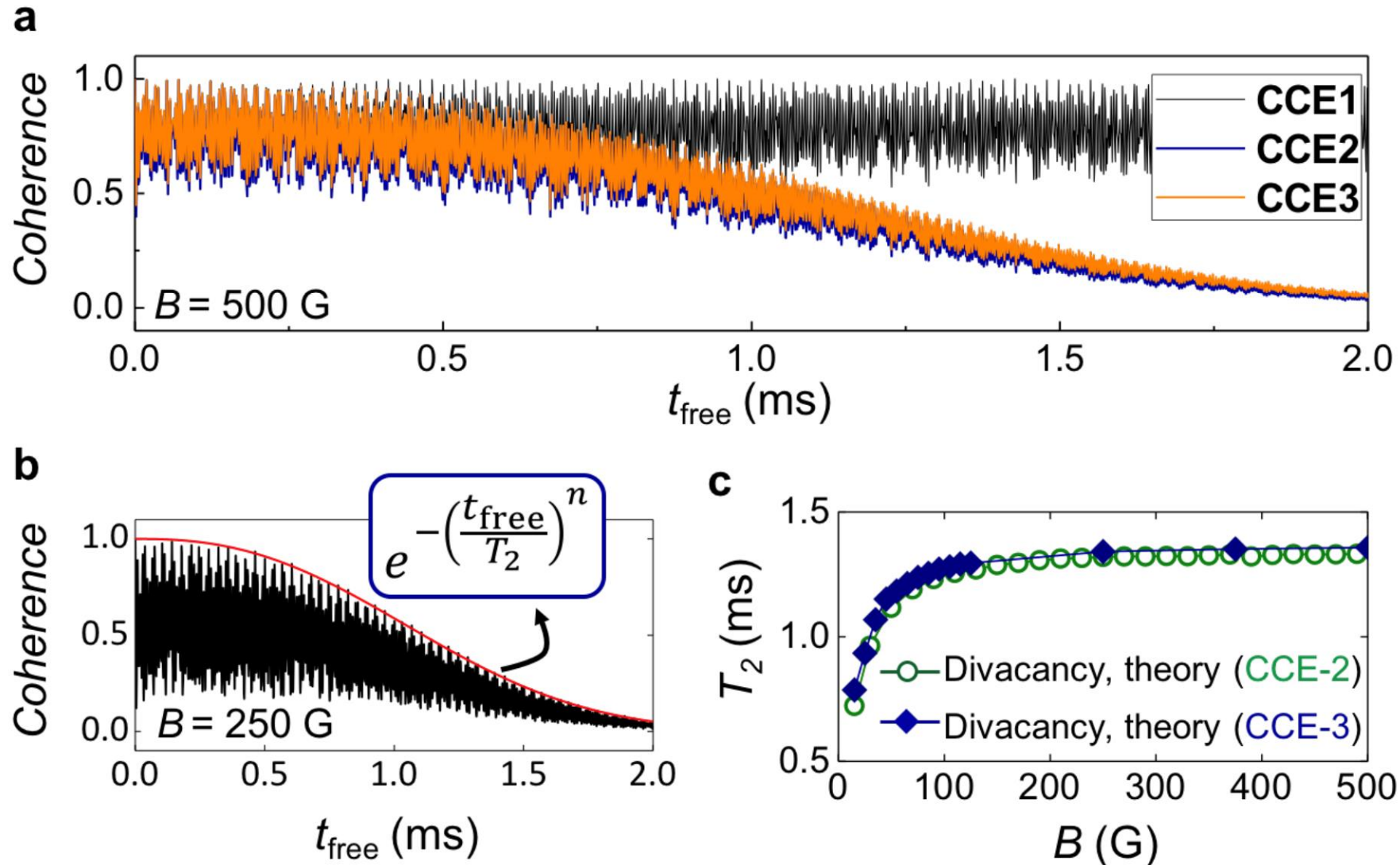
CCE ansatz:

$$L(t) = \prod_n L_n(t) \qquad L_n(t) = \prod_{j \in C_n} \tilde{l}_j^{(n)}(t)$$

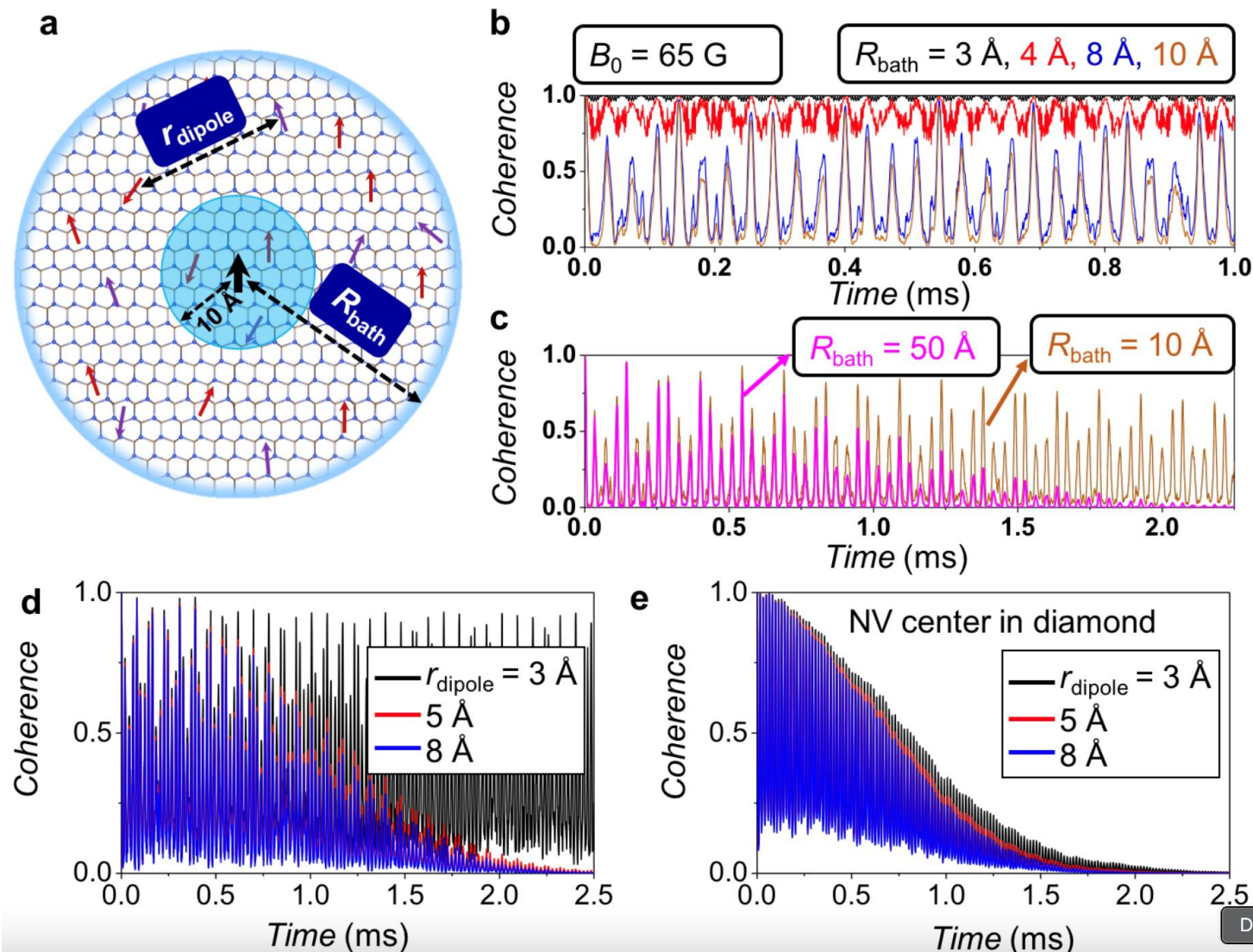
$$\tilde{l}_j^{(n)} = \frac{\text{Tr}(\sigma_+ \text{Tr}_{\text{bath}}(\varrho_j^{(n)}))}{l^{(0)} \prod_{p \in C_{1,j}} \tilde{l}_p^{(1)} \cdots \prod_{q \in C_{n-1,j}} \tilde{l}_q^{(n-1)}}$$



# Introduction of the CCE method



# Introduction of the CCE method



# Nuclear spins as resources

- Adjacent nuclear spins can be addressed by the NV center
  - Additional spin qubits with long coherence time
  - Trend:
    - electron spin: means of nuclear spin initialization, control and read-out.
    - nuclear spins: multi-qubit quantum hardware.

## Mapping a 50-spin-qubit network through correlated sensing

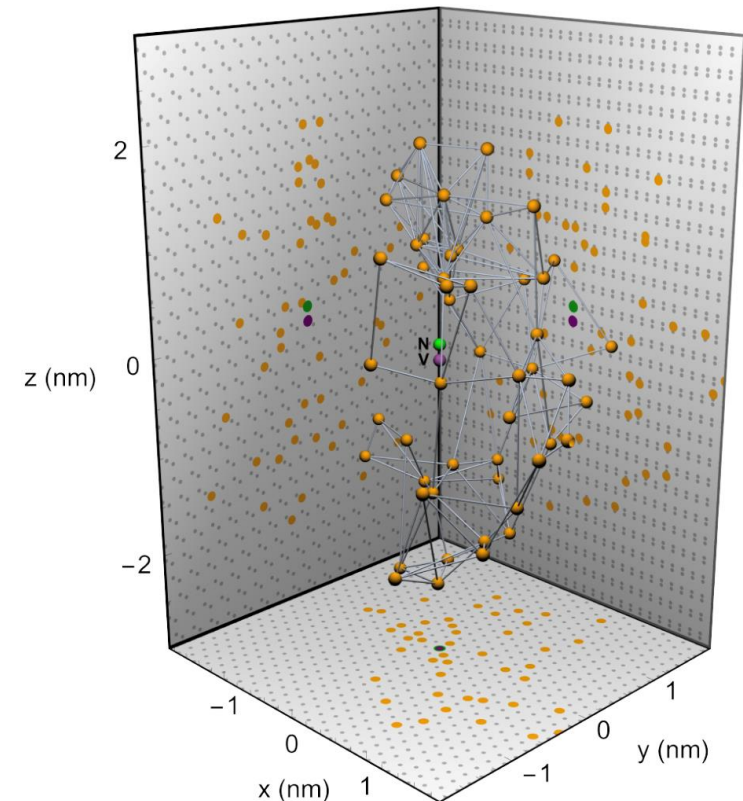
G.L. van de Stolpe<sup>1,2</sup>, D. P. Kwiatkowski<sup>1,2</sup>, C.E. Bradley<sup>1,2</sup>, J. Randall<sup>1,2</sup>, S. A. Breitweiser<sup>3</sup>, L. C. Bassett<sup>3</sup>, M. Markham<sup>4</sup>, D.J. Twitchen<sup>4</sup>, and T.H. Taminiau<sup>1,2</sup>

<sup>1</sup>*QuTech, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands*

<sup>2</sup>*Kavli Institute of Nanoscience Delft, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands*

<sup>3</sup>*Quantum Engineering Laboratory, Department of Electrical and Systems Engineering, University of Pennsylvania, 200 South 33rd Street, Philadelphia, PA 19104, USA and*

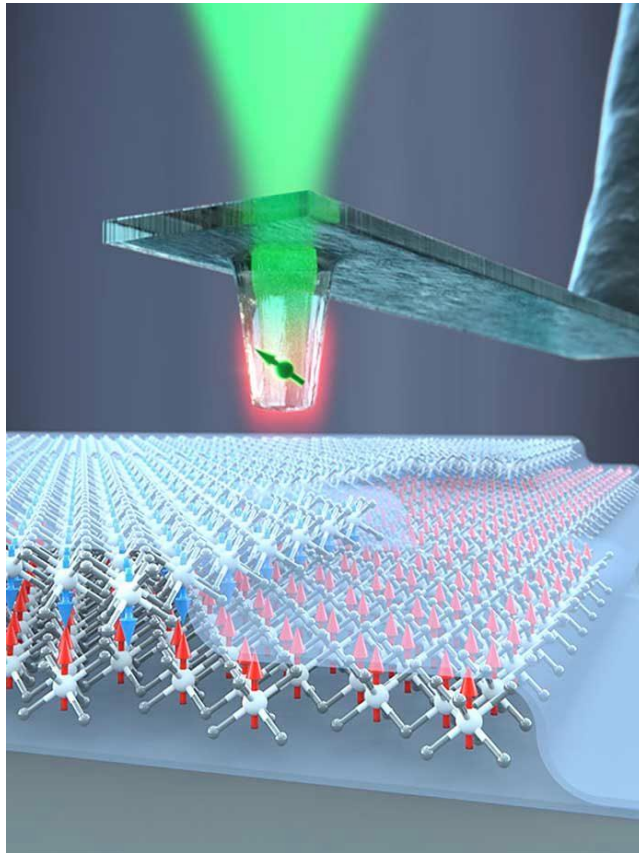
<sup>4</sup>*Element Six Innovation, Fermi Avenue, Harwell Oxford, Didcot, Oxfordshire OX11 0QR, United Kingdom*



# Part II.

Interesting experiments and papers

# Quantum sensing with NV center



Single NV center  
High spatial resolution

Nanoscale probe  
Nature **455** 648 (2008)

Ensemble of NV centers



Very high precision, low spatial resolution

# Sensitivity for AC magneometry

$\eta$  ( $\tau_{\text{full}} = 1$  s) represents the smallest signal field that can be detected with SNR = 1 in 1 second of interrogation time.

$$\eta \approx \frac{\pi}{2} \frac{\hbar}{g_e \mu_B} \frac{1}{\sqrt{N \tau_{\text{full}}}} \frac{1}{e^{-\tau_{\text{full}}/(k^s T_2)^p}} \times \sqrt{1 + \frac{1}{C^2 n_{\text{avg}}}} \sqrt{\frac{t_I + \tau_{\text{full}} + t_R}{\tau_{\text{full}}}}$$

Large  $N \Rightarrow$  sub femto tesla sensitivity

REPORT

QUANTUM MEASUREMENT

Submillihertz magnetic spectroscopy performed with a nanoscale quantum sensor

Simon Schmitt,<sup>1</sup> Tuvia Gefen,<sup>2</sup> Felix M. Stürner,<sup>1</sup> Thomas Unden,<sup>1</sup> Gerhard Wolff,<sup>1</sup> Christoph Müller,<sup>1</sup> Jochen Scheuer,<sup>1,3</sup> Boris Naydenov,<sup>1,3</sup> Matthew Markham,<sup>4</sup> Sebastien Pezzagna,<sup>5</sup> Jan Meijer,<sup>5</sup> Ilai Schwarz,<sup>3,6</sup> Martin Plenio,<sup>3,6</sup> Alex Retzker,<sup>2</sup> Liam P. McGuinness,<sup>1\*</sup> Fedor Jelezko<sup>1,3</sup>

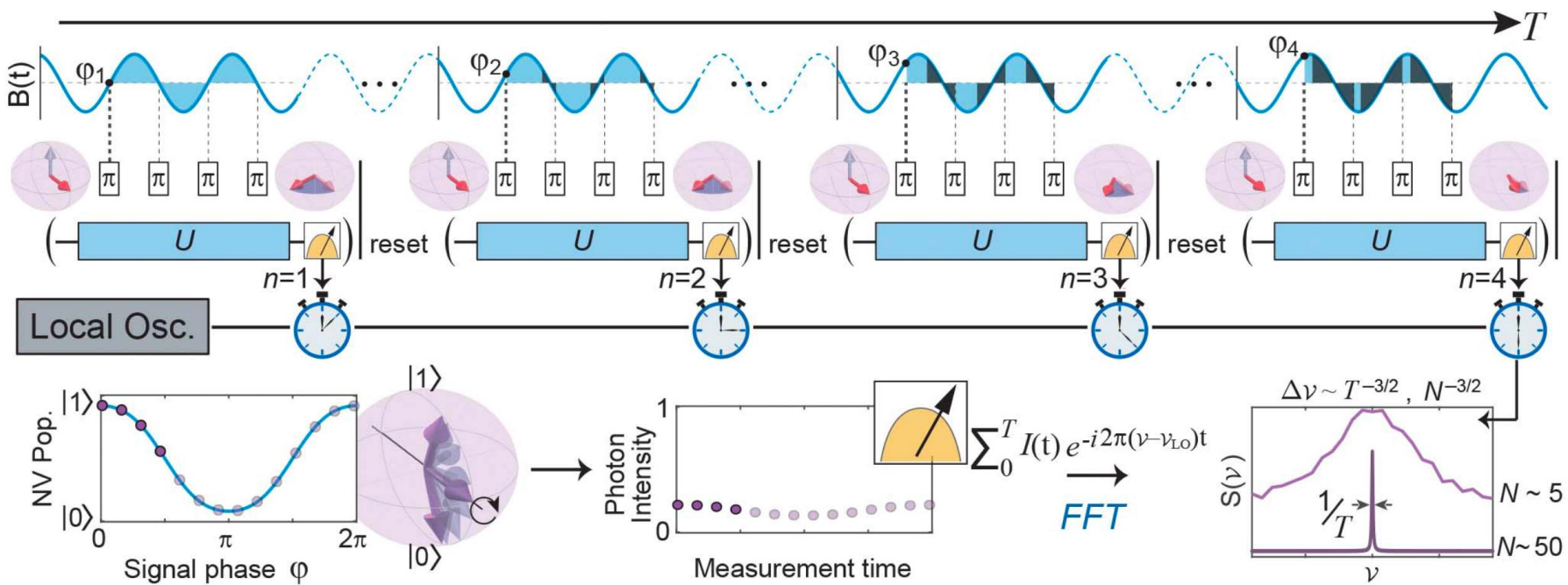
QUANTUM MEASUREMENT

Quantum sensing with arbitrary frequency resolution

J. M. Boss,<sup>\*</sup> K. S. Cujia,<sup>\*</sup> J. Zopes, C. L. Degen<sup>†</sup>

*Science* **356**, 832–837 (2017)

*Science* **356**, 837–840 (2017)

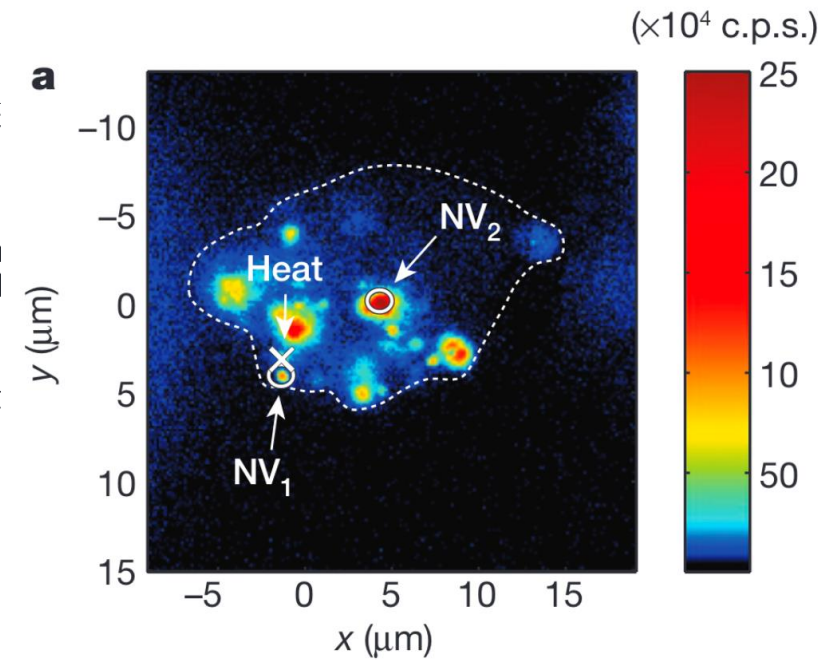


# Can we measure temperature in living cells?

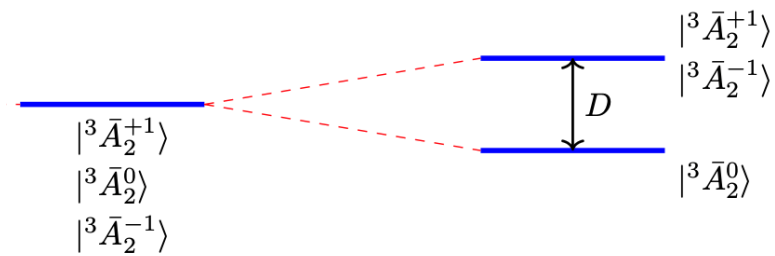
## LETTER

### Nanometre-scale thermometry in :

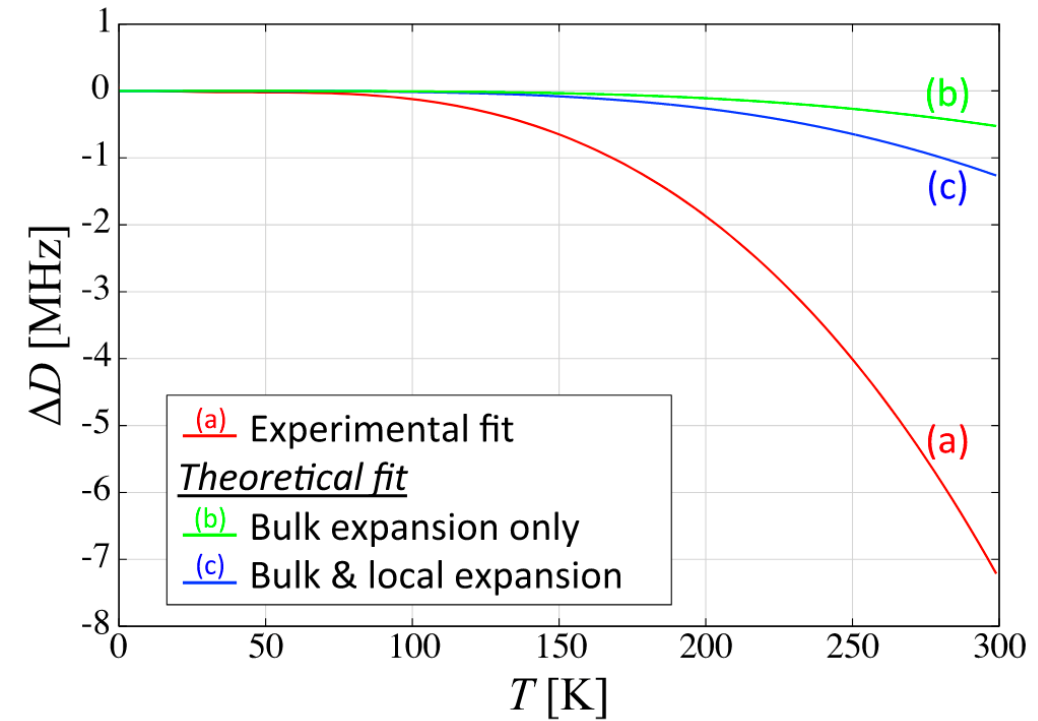
G. Kucsko<sup>1\*</sup>, P. C. Maurer<sup>1\*</sup>, N. Y. Yao<sup>1</sup>, M. Kubo<sup>2</sup>, H. J. Noh<sup>3</sup>, P. K. Lo<sup>4</sup>, H. Park<sup>1,2,3</sup> &



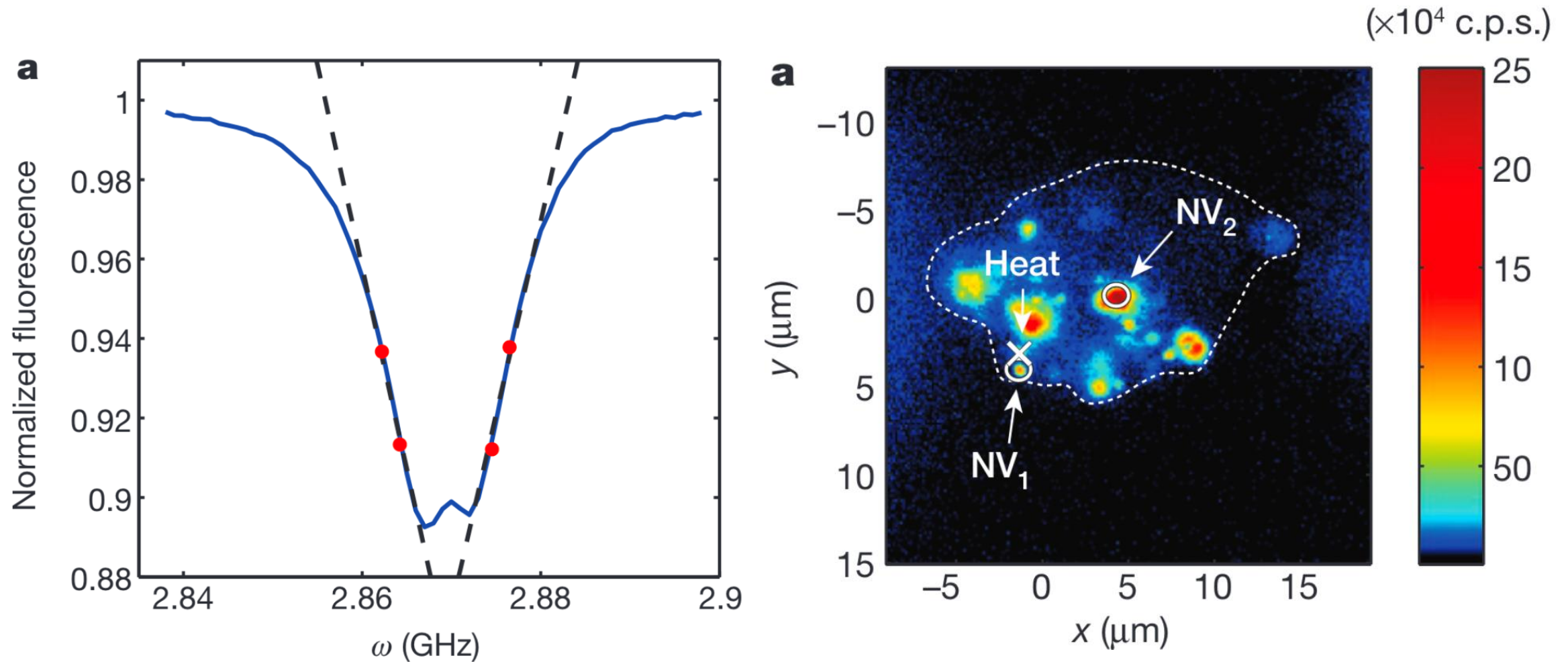
# Temperature dependence of



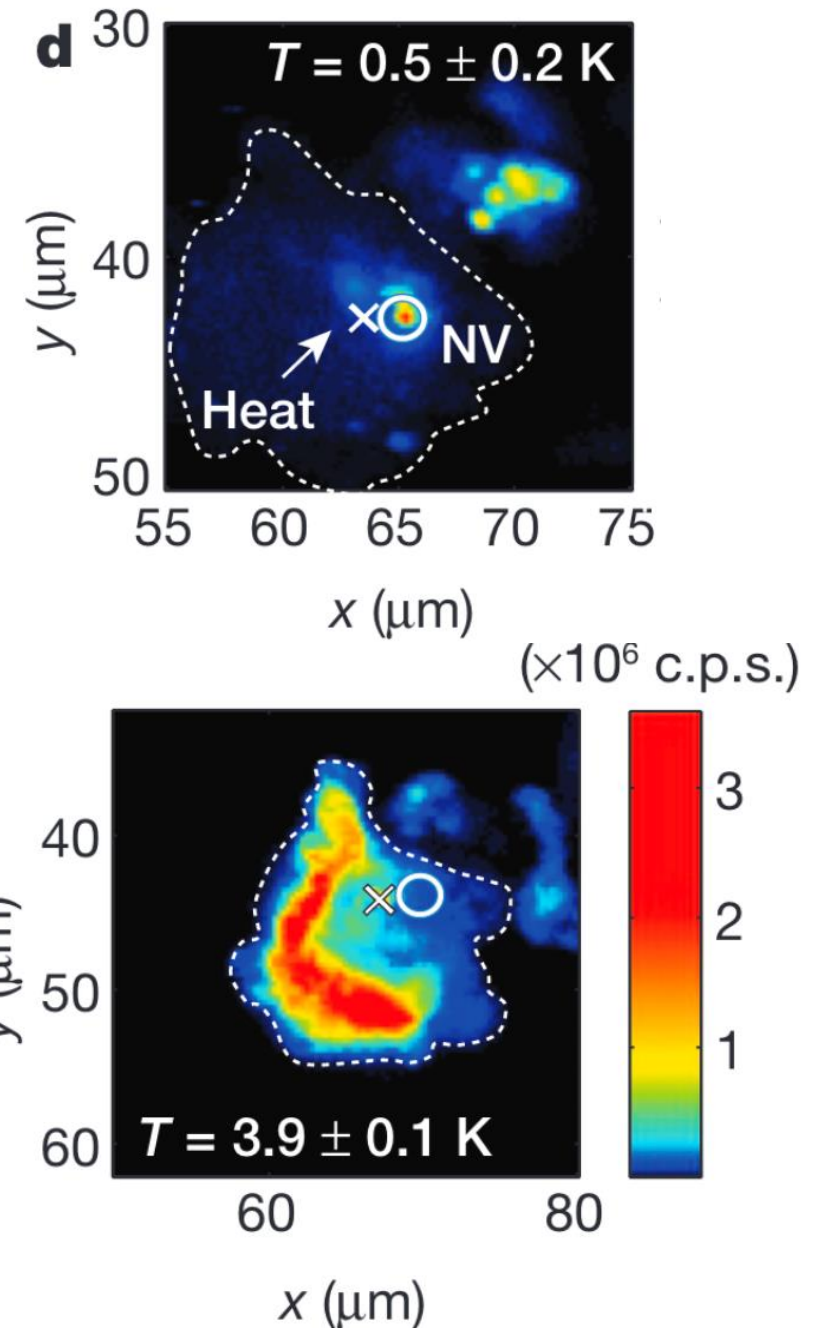
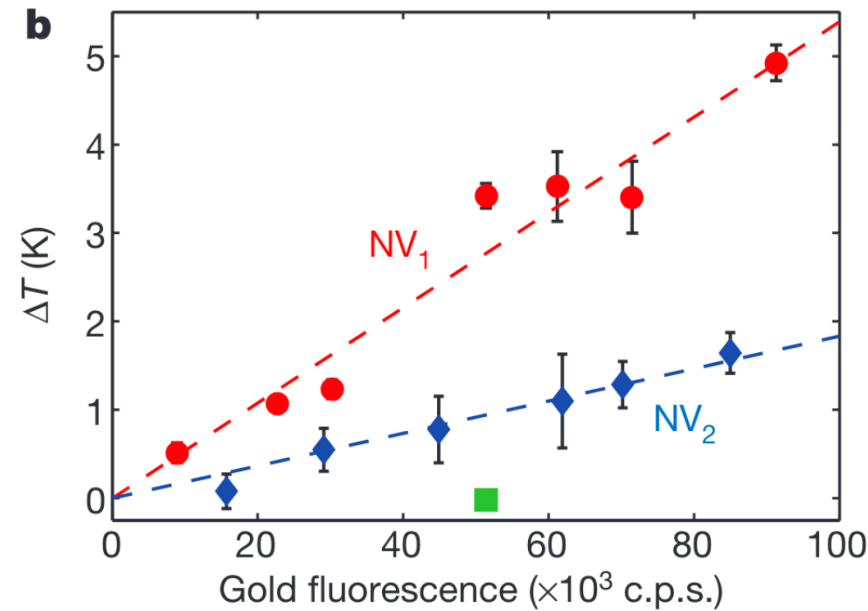
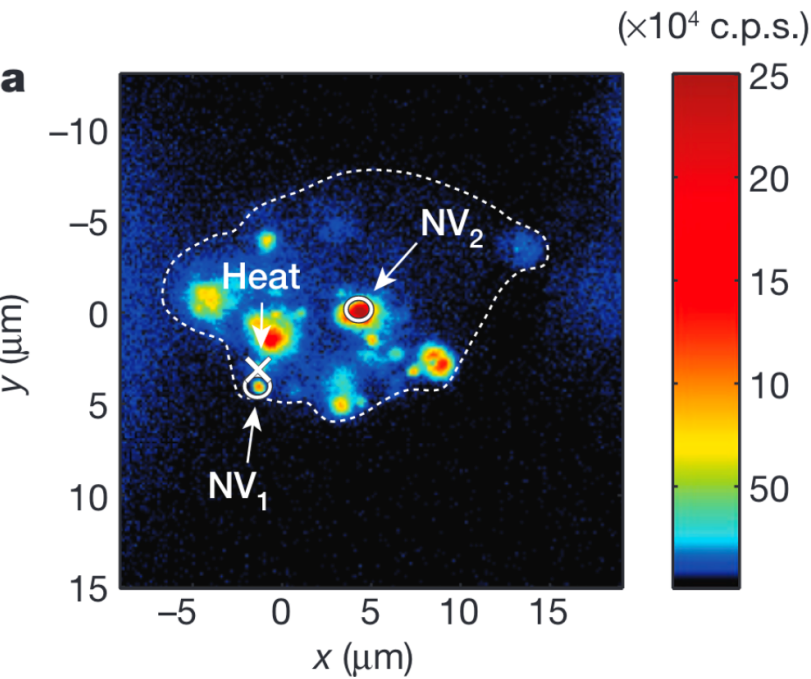
$$h_{ss} = -\frac{\mu_0}{4\pi} \frac{g^2 \beta^2}{r^3} (3(\mathbf{s}_1 \cdot \hat{r})(\mathbf{s}_2 \cdot \hat{r}) - \mathbf{s}_1 \cdot \mathbf{s}_2)$$



# Use the PL intensity variation detect change of the temperature



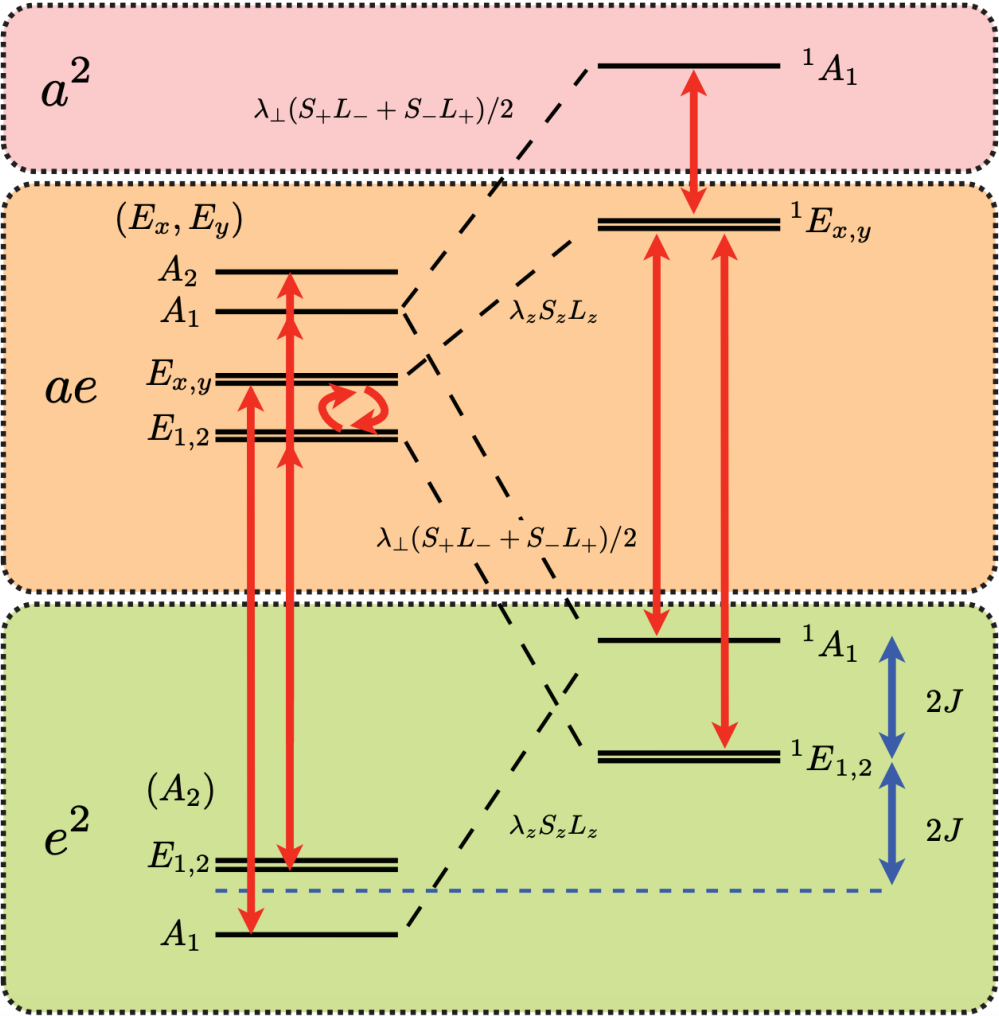
Increased heating is detected in the cell until it popped...



## Loophole-free Bell inequality violation using electron spins separated by 1.3 kilometres

B. Hensen<sup>1,2</sup>, H. Bernien<sup>1,2†</sup>, A. E. Dréau<sup>1,2</sup>, A. Reiserer<sup>1,2</sup>, N. Kalb<sup>1,2</sup>, M. S. Blok<sup>1,2</sup>, J. Ruitenber<sup>1,2</sup>, R. F. L. Vermeulen<sup>1,2</sup>, R. N. Schouten<sup>1,2</sup>, C. Abellán<sup>3</sup>, W. Amaya<sup>3</sup>, V. Pruneri<sup>3,4</sup>, M. W. Mitchell<sup>3,4</sup>, M. Markham<sup>5</sup>, D. J. Twitchen<sup>5</sup>, D. Elkouss<sup>1</sup>, S. Wehner<sup>1</sup>, T. H. Taminiau<sup>1,2</sup> & R. Hanson<sup>1,2</sup>

# One way of creating spin-photon entanglement with the NV center



Optical selection rules can be derived from the many-body states.

| $\hat{e}$  | $A_1$            | $A_2$            | $E_1$            | $E_2$            | $E_x$     | $E_y$     | $\hat{e}$ | $^1E_x$   | $^1E_y$   | $\hat{e}$ | $^1A_1$   |
|------------|------------------|------------------|------------------|------------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| $^3A_{2-}$ | $\hat{\sigma}_+$ | $\hat{\sigma}_+$ | $\hat{\sigma}_-$ | $\hat{\sigma}_-$ |           |           | $^1A_1$   | $\hat{x}$ | $\hat{y}$ | $^1E_1$   | $\hat{x}$ |
| $^3A_{20}$ |                  |                  |                  |                  | $\hat{y}$ | $\hat{x}$ | $^1E_1$   | $\hat{x}$ | $\hat{y}$ | $^1E_2$   | $\hat{y}$ |
| $^3A_{2+}$ | $\hat{\sigma}_-$ | $\hat{\sigma}_-$ | $\hat{\sigma}_+$ | $\hat{\sigma}_+$ |           |           | $^1E_2$   | $\hat{y}$ | $\hat{x}$ |           |           |

$\hat{\sigma}_{\pm} = \hat{x} \pm i\hat{y}$

[1] New Journal of Physics **13** 025025 (2011).

Linearly polarized photons

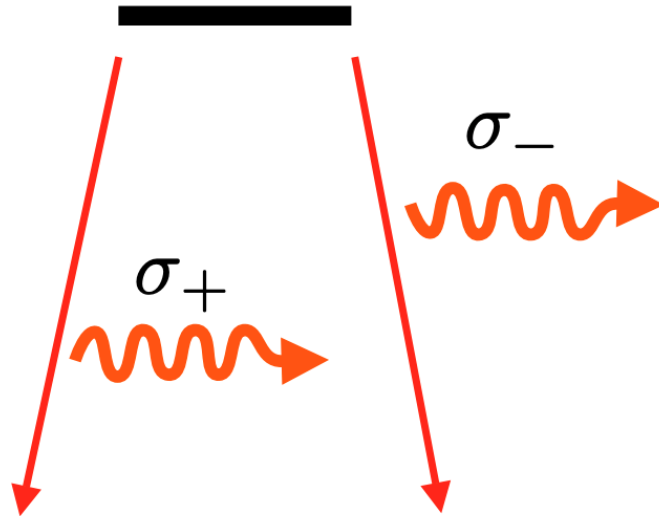
Circularly polarized photons

$A_2$ : no non-radiative decay, selectively coupled with the ground state through circularly polarized photon emission.

# Lambda scheme

## Spin-photon entanglement generation

$$|A_2\rangle = |E_+\rangle \otimes |\beta\beta\rangle + |E_-\rangle \otimes |\alpha\alpha\rangle$$

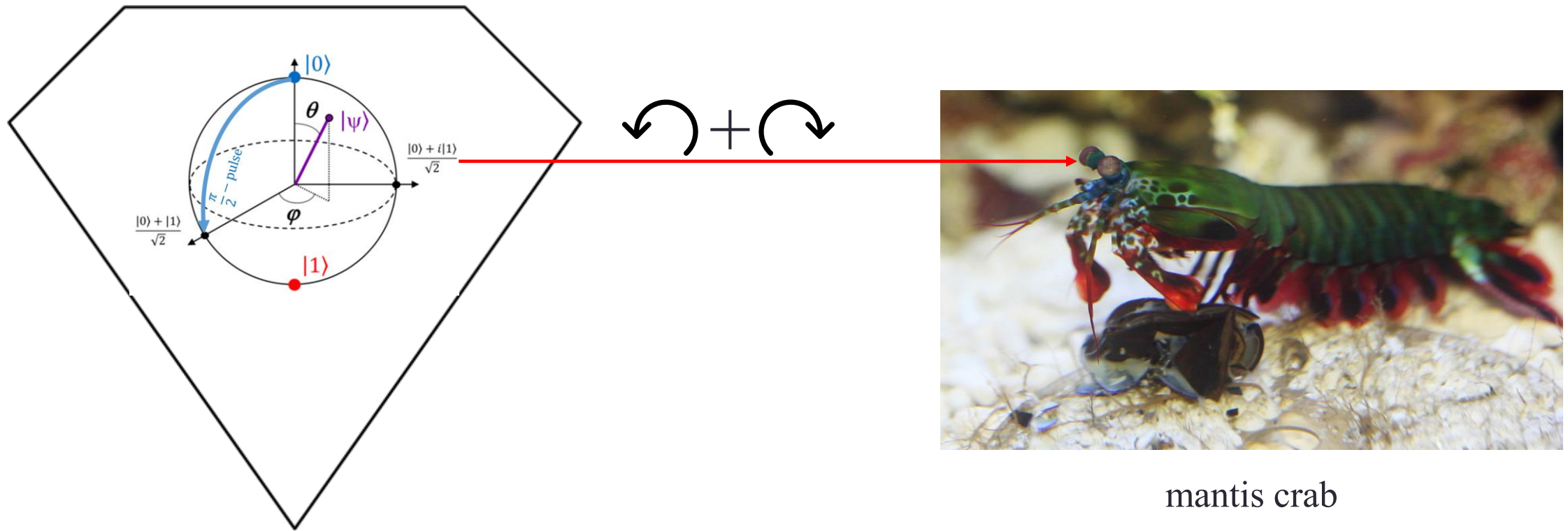


$$|^3A_{2-}\rangle = |E_0\rangle \otimes |\beta\beta\rangle \quad |E_0\rangle \otimes |\alpha\alpha\rangle = |^3A_{2+}\rangle$$

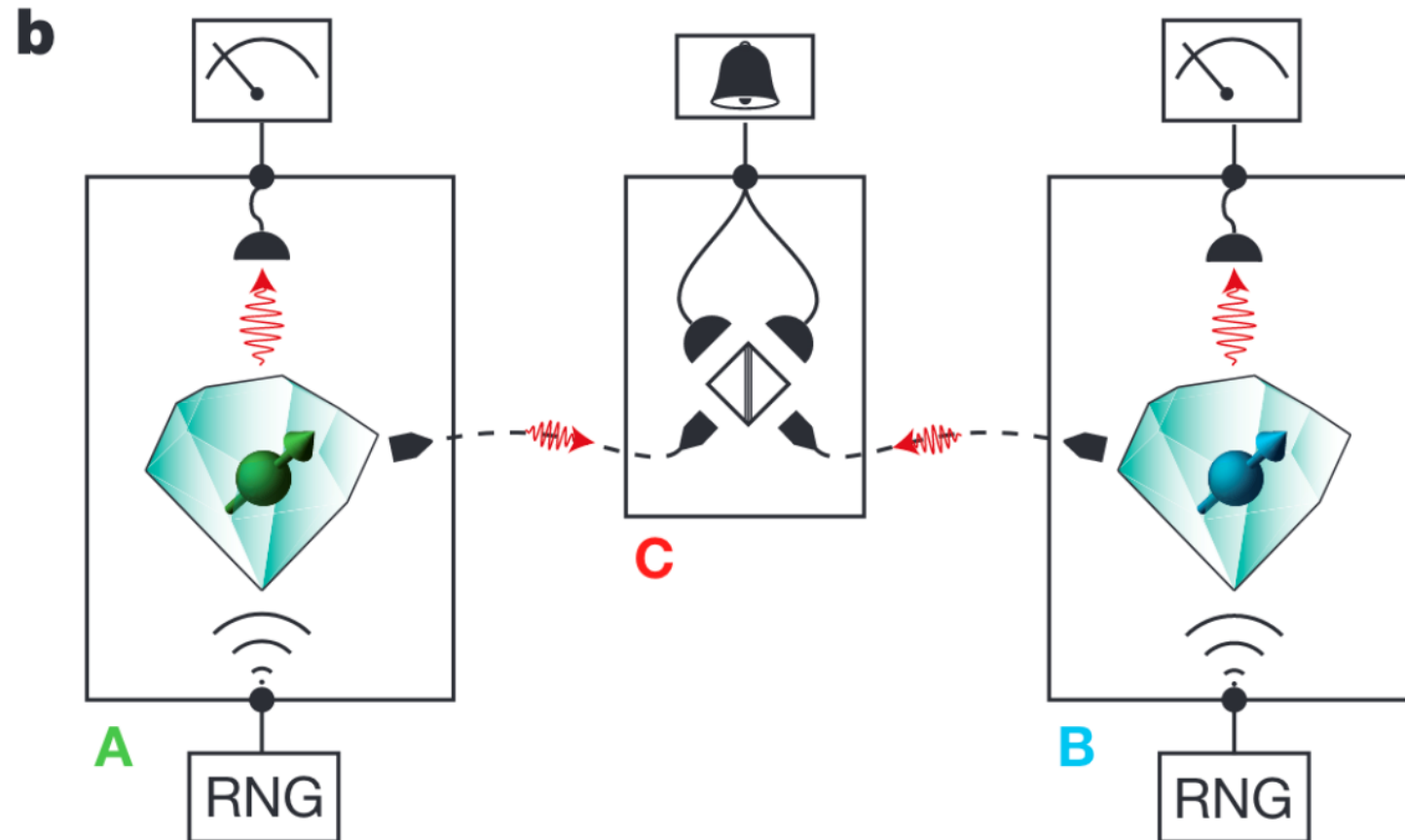
$$\frac{1}{\sqrt{2}} (|+1\rangle \otimes |\sigma_-\rangle + |-1\rangle \otimes |\sigma_+\rangle)$$

# Schrödinger's cat problem 2.0

Low temperature NV emission

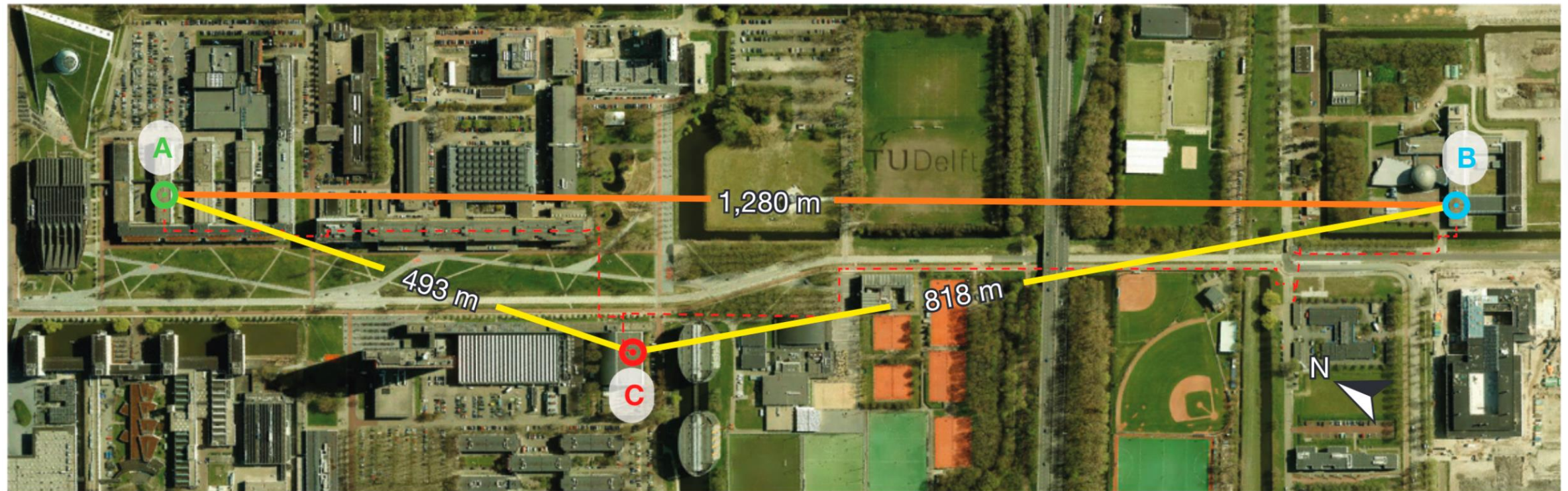


# Entanglement swap via a beam splitter and photon detection



- Entangled photons are arriving to C from A and B.
- Entangle through a beam splitter  $\Rightarrow$  four particle entanglement
- Photons are measured, which entangle the A and B.
- Bell inequality violation tested.

The tests are carried out faster than light could travel from A to B.

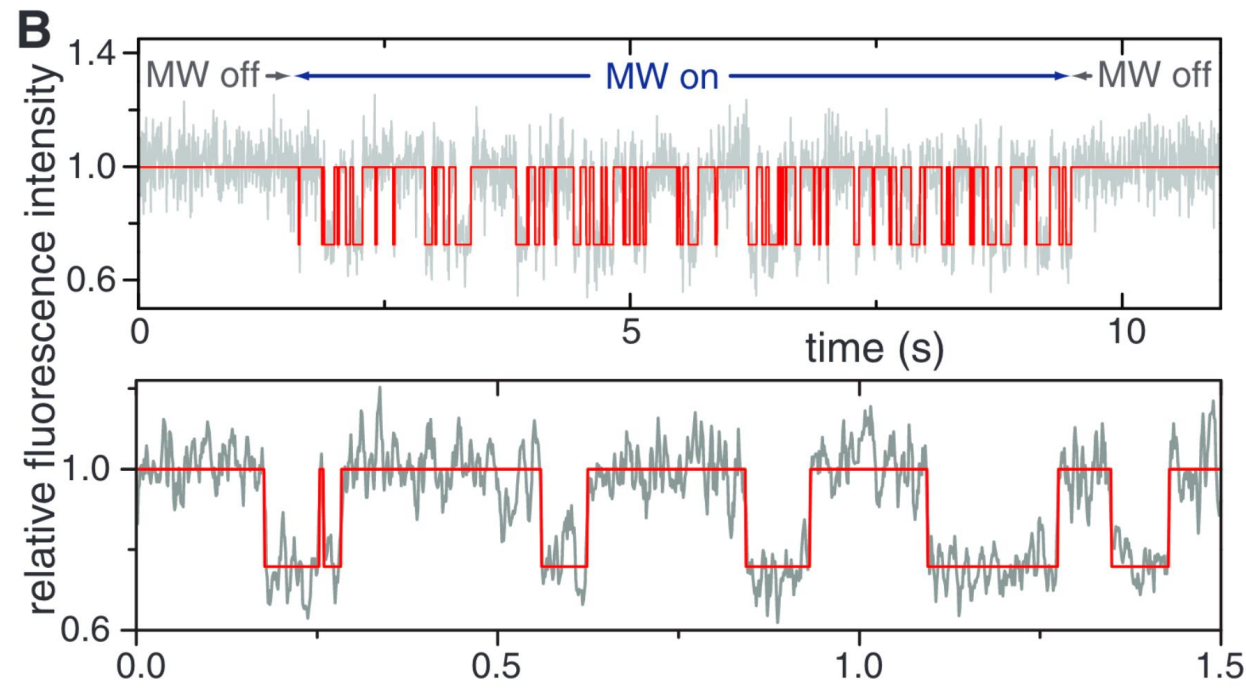


HOME &gt; SCIENCE &gt; VOL. 329, NO. 5991 &gt; SINGLE-SHOT READOUT OF A SINGLE NUCLEAR SPIN

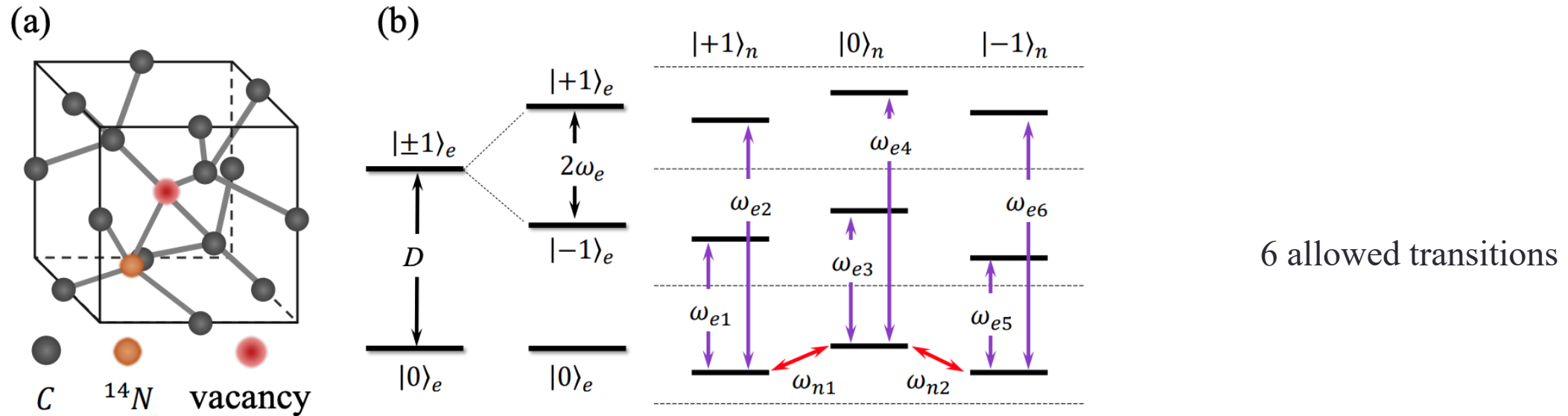
🔒 | REPORT



# Single-Shot Readout of a Single Nuclear Spin

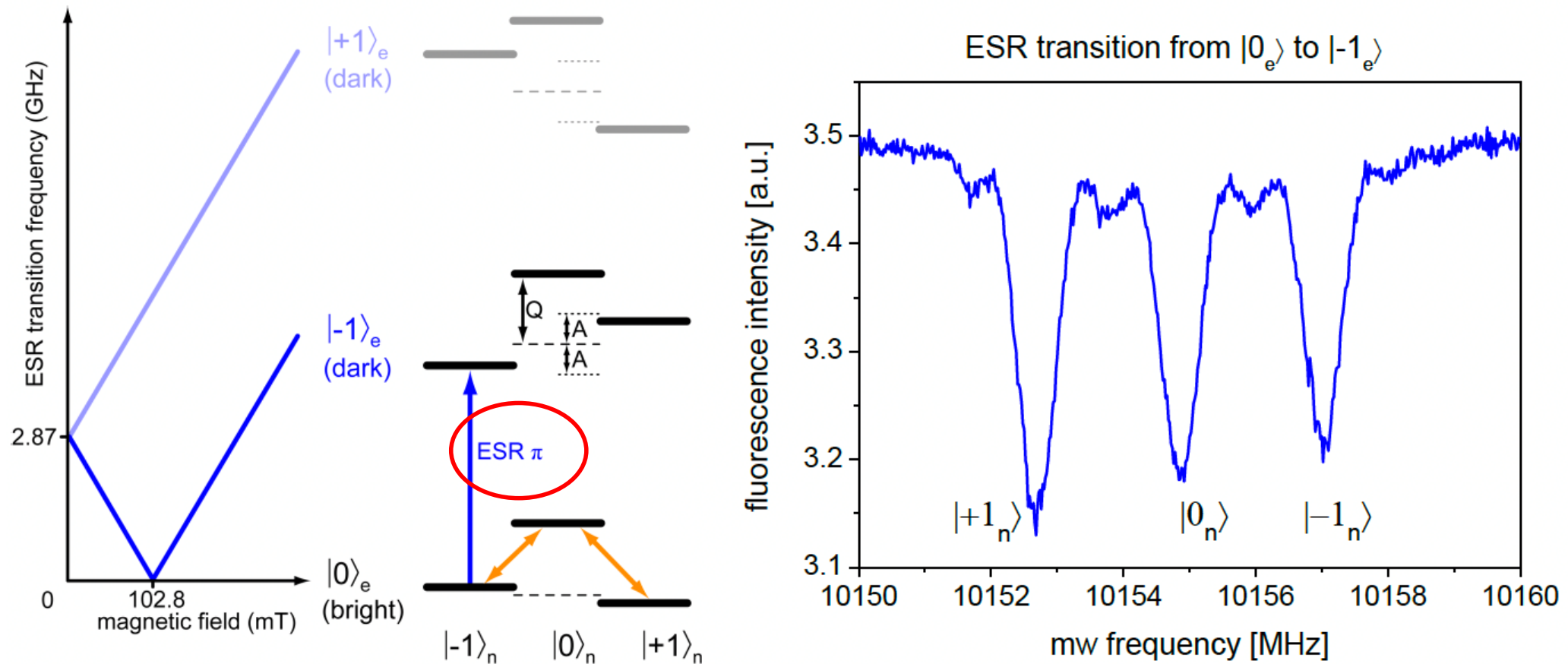
PHILIPP NEUMANN, JOHANNES BECK, MATTHIAS STEINER, FLORIAN REMPP, HELMUT FEDDER, PHILIP R. HEMMER, JÖRG WRACHTRUP, AND FEDOR JELEZKO [Authors Info &](#)[Affiliations](#)

# NV is it as two qutrit system



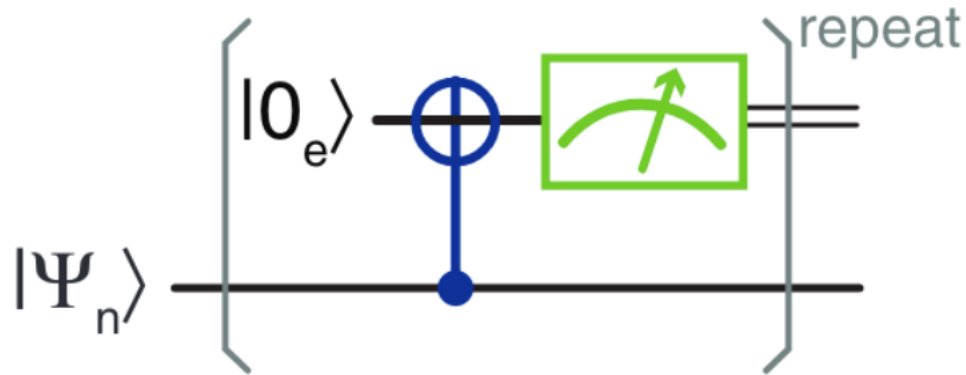
$$H = \underbrace{D\hat{S}_z^2 + g_e\mu_B B_z \hat{S}_z}_{H_e} + \underbrace{\hat{\underline{S}} \cdot \hat{\underline{A}} \cdot \hat{\underline{I}}}_{H_A} + \underbrace{Q\hat{I}_z^2 + g_n\mu_n B_z \hat{I}_z}_{H_n}$$

# Nuclear spin resolved ODMR spectra

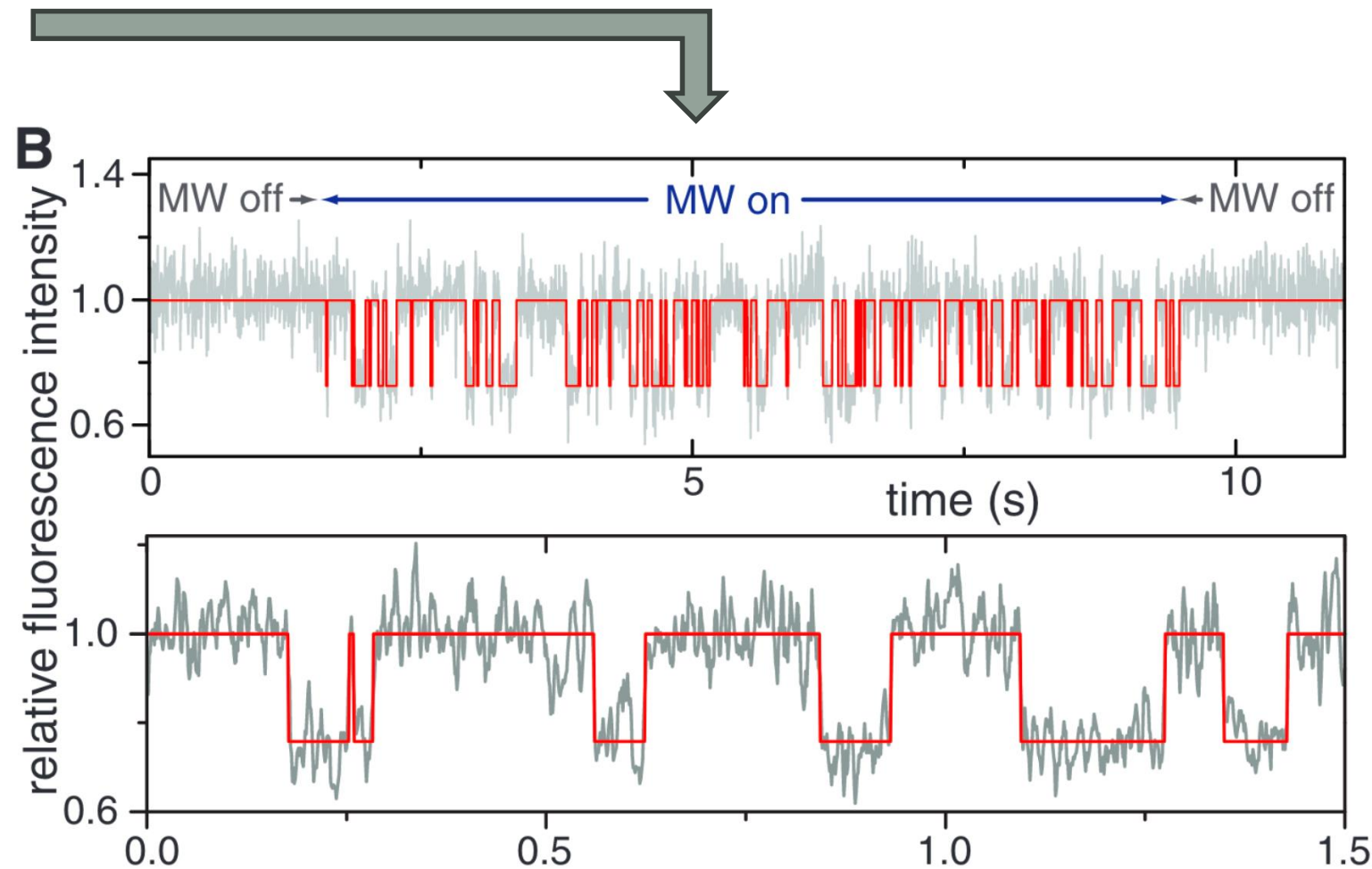


We can use these transitions to implement CNOT operation.

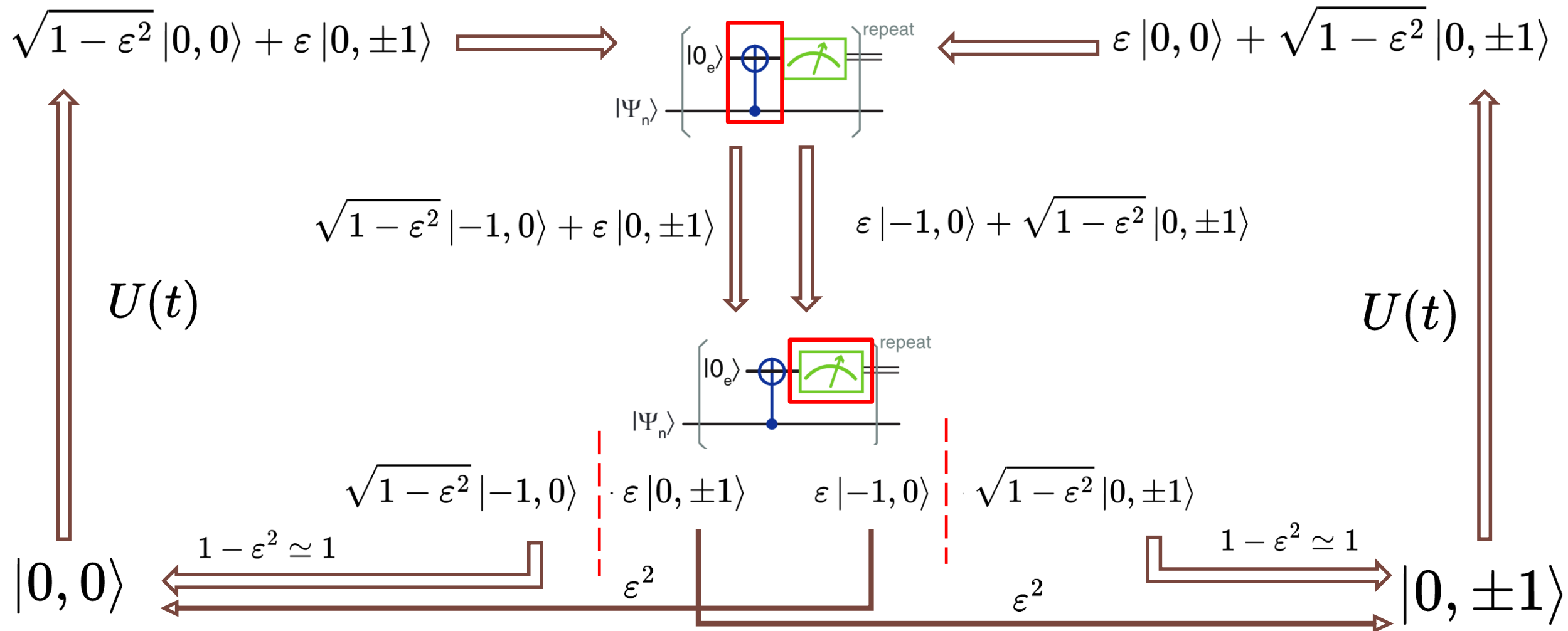
# Implement “fast” indirect measurement of nuclear spin states



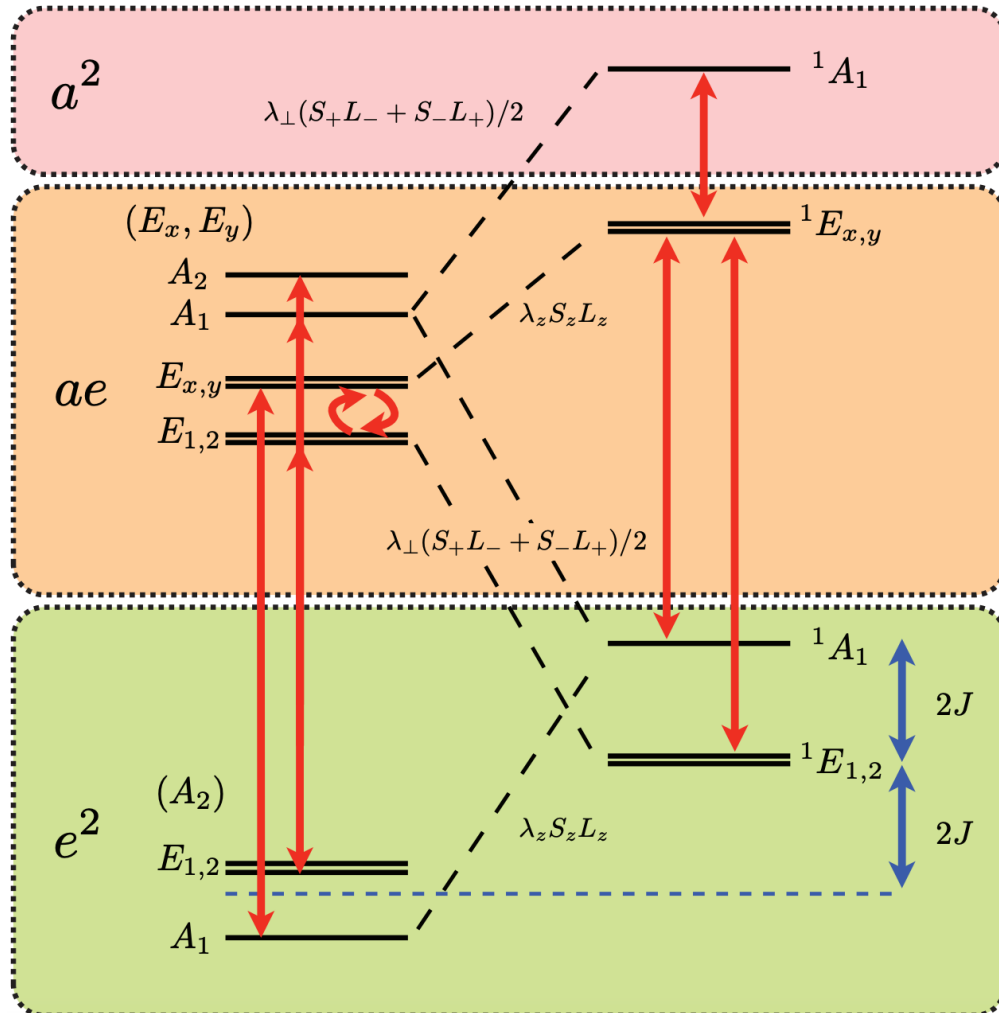
Approaching the quantum Zeno limit.



# Two loops of time evolution



# What we can learn from the optical cycle



$$\hat{M}_1 = |m_S = 0\rangle\langle m_S = 0|$$

$$\hat{M}_2 = |m_S = 0\rangle\langle m_S = \pm 1|$$

Optical excitation coherent  $U(t)$

Spontaneous emission projective:  $M_1$

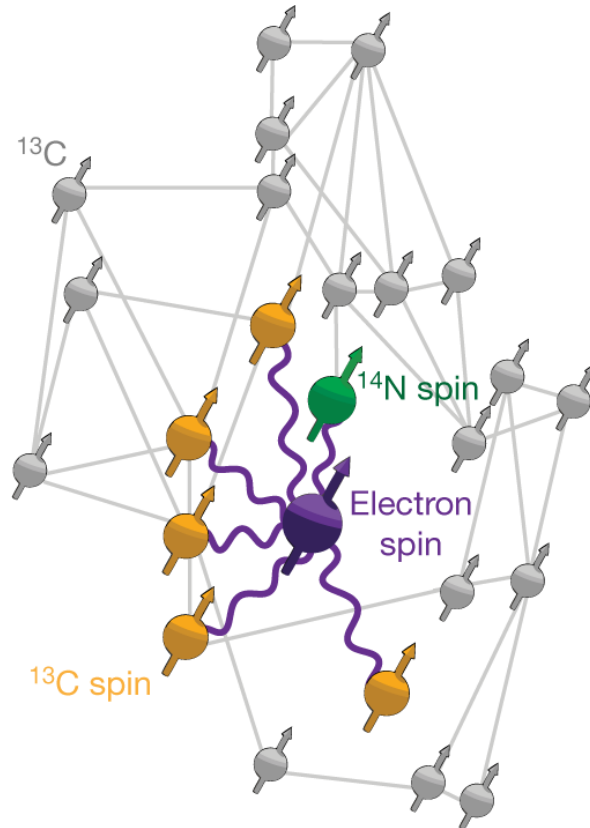
Non-radiative decay projective:  $M_2$

# PART III.

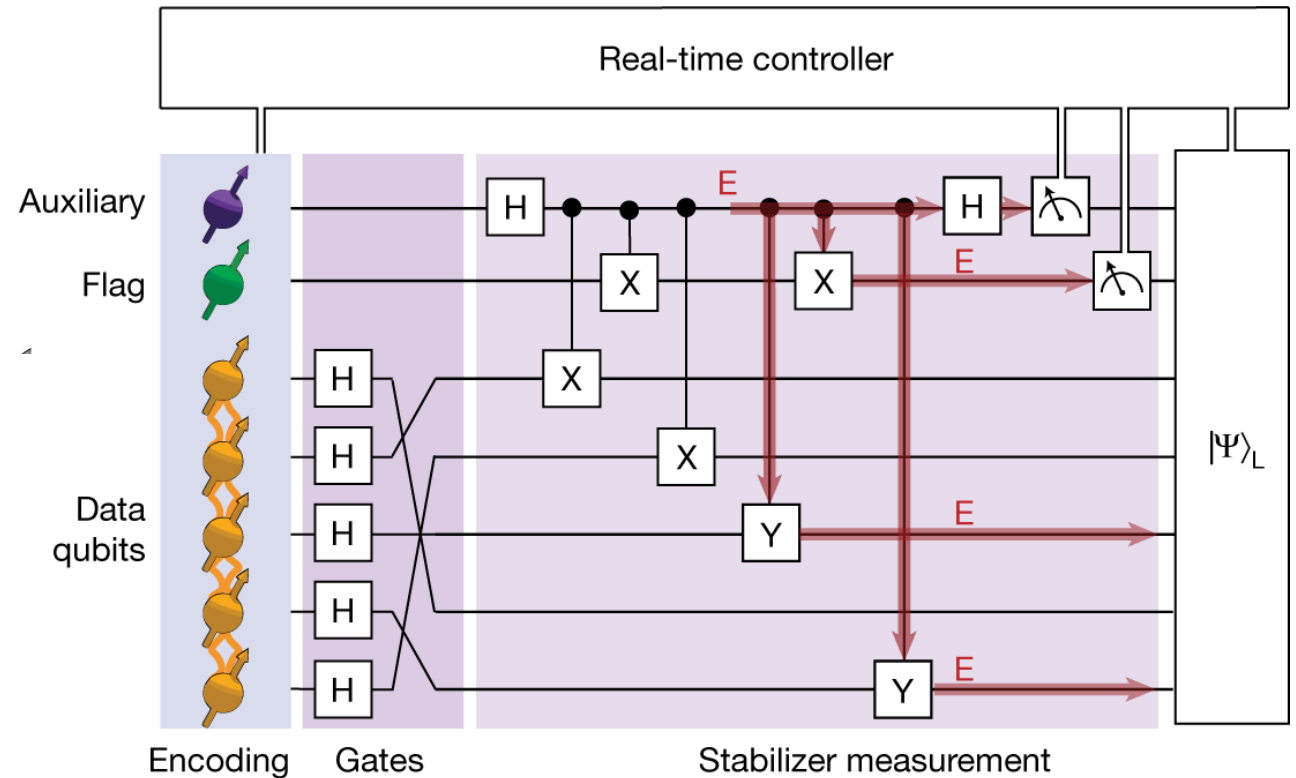
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Perspectives and challenges in QC and QRC

# 5-20 qubit quantum computer at room temperature



1 NV centrum + néhány magspin kubit

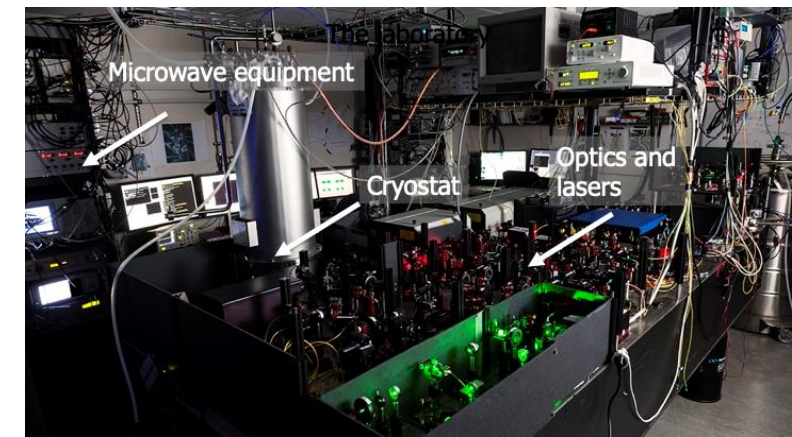
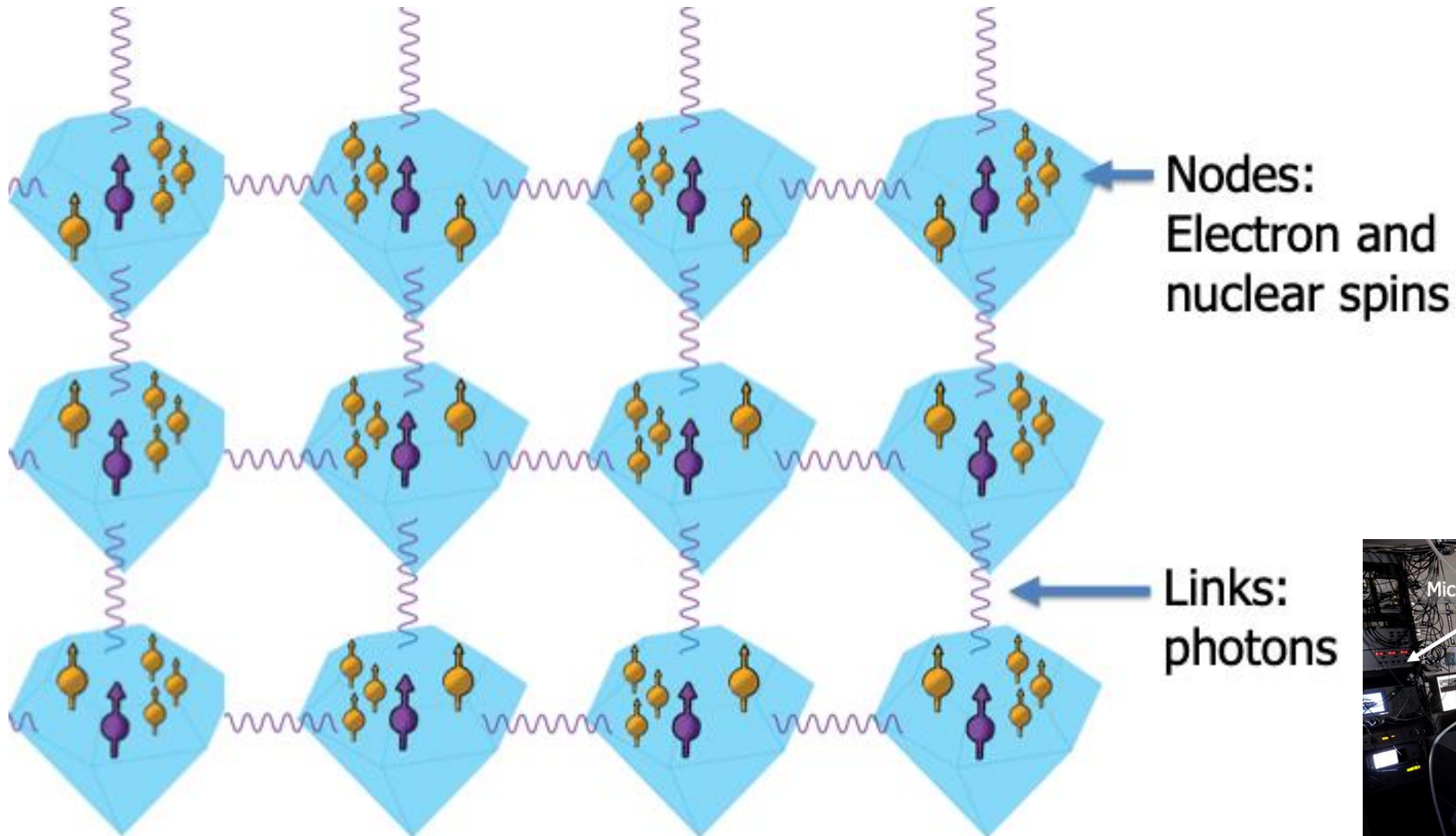


## Fault-tolerant operation of a logical qubit in a diamond quantum processor

M. H. Abobeih, Y. Wang, J. Randall, S. J. H. Loenen, C. E. Bradley, M. Markham, D. J. Twitchen, B. M. Terhal & T. H. Taminiau [✉](#)

*Nature* **606**, 884–889 (2022) | [Cite this article](#)

# Possibility of scaling?



# Potential to Q(R)C

- Scalling is as hard as diamond.
  - Atomic-scale fabrication in hard materials is difficult.
- Flying qubits must be involved
  - Photon,
  - Phonons
  - Magnons
  - Electrons
- These will be / are the main sources of decoherence
- Noise-tolerant QC applications are required, such as QRC.