Computational Exploration of Diamond NV$^-$ Qubits via Quantum Optimal Control Theory

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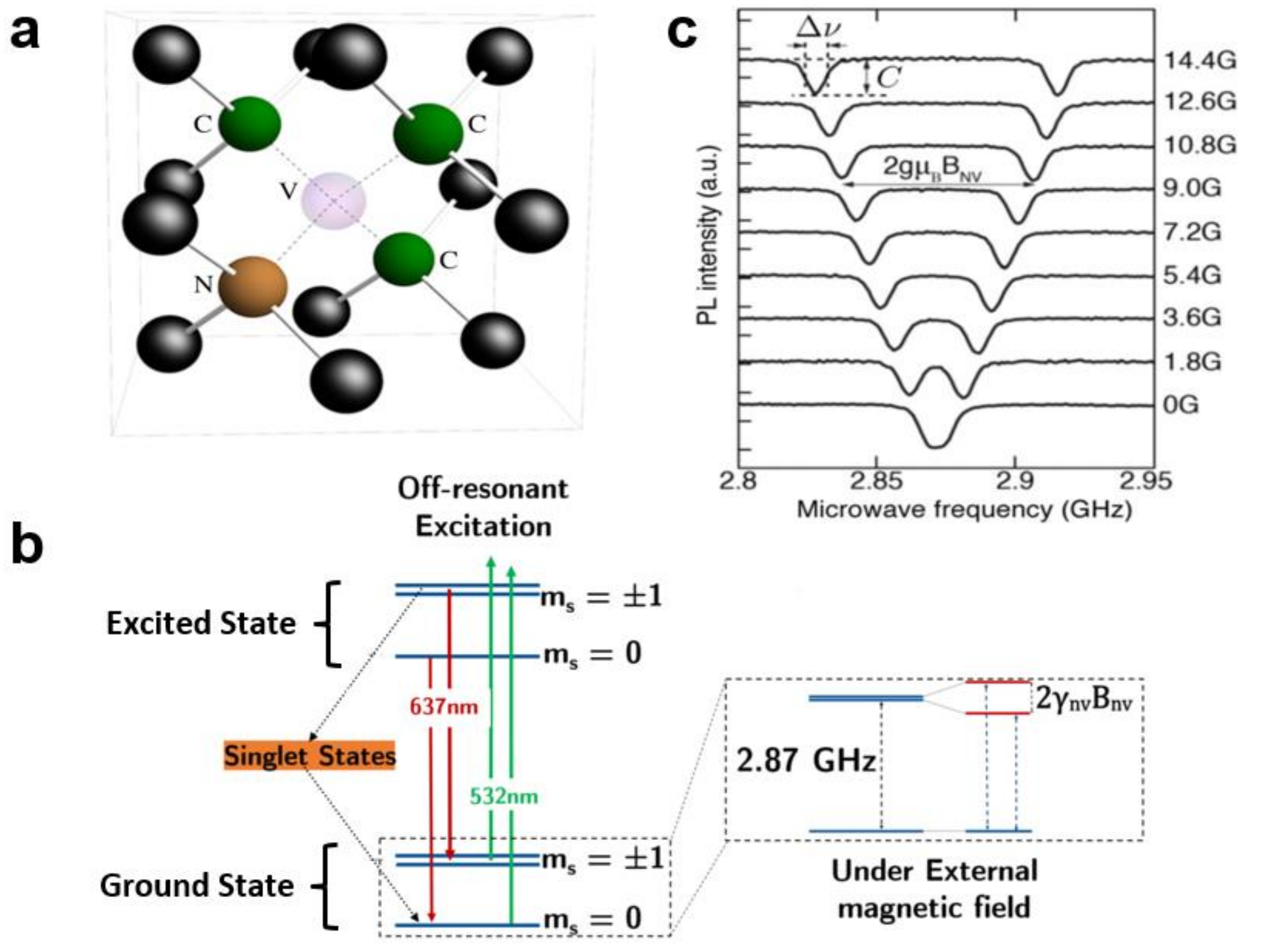
The Diamond NV$^-$ Center

- Negatively charged nitrogen vacancy (NV$^-$) centers in diamond (**a**) are a promising platform for qubits, as they are stable at room temperature, optically active, controllable via radio frequency pulses, and can act as an effective 2-state quantum system.
- The NV$^-$ electron is spin-1, with a fine structure splitting of ~2.87 GHz between the m=0 and m=±1 spin sublevels. The m=±1 states can be further split by an applied magnetic field (**b**). Via optical pumping, the NV$^-$ system can be initialized into the m=0 state, and Zeeman splitting (**c**) of the m=±1 states is observable via optically detected magnetic resonance (ODMR).



Quantum Optimal Control (QOC) Theory

- NV-based spin registers can be used as qubits at room temperature and have been shown to have long coherence times. These properties make it a promising candidate for quantum computing.
- However, the complex system are difficult to control in realistic environments.
- Multi-qubit registers often experience crosstalk errors while implementing gates, as well as the full register decohering.
- These errors bring in the need for QOC to numerically optimize pulse sequences

Gradient Ascent Pulse Engineering (GRAPE)

- We chose to use a QuTIP package implementing GRAPE for this project
- In a closed quantum system, time evolution between states is described by a unitary transformation. The time dependent Schrodinger equation can be written as shown below where the Hamiltonian is split up into the drift and control terms and the u(t) terms are controllable amplitudes that vary with time.
- The GRAPE algorithm then optimizes the fidelity of the target state using a
- "hill climbing" method.

$$H(t) = H_0 + \sum_{j=1} u_j(t)H_j \qquad H(t) \approx H(t_k) = H_0 \sum_{j=1} u_{jk}H_j$$

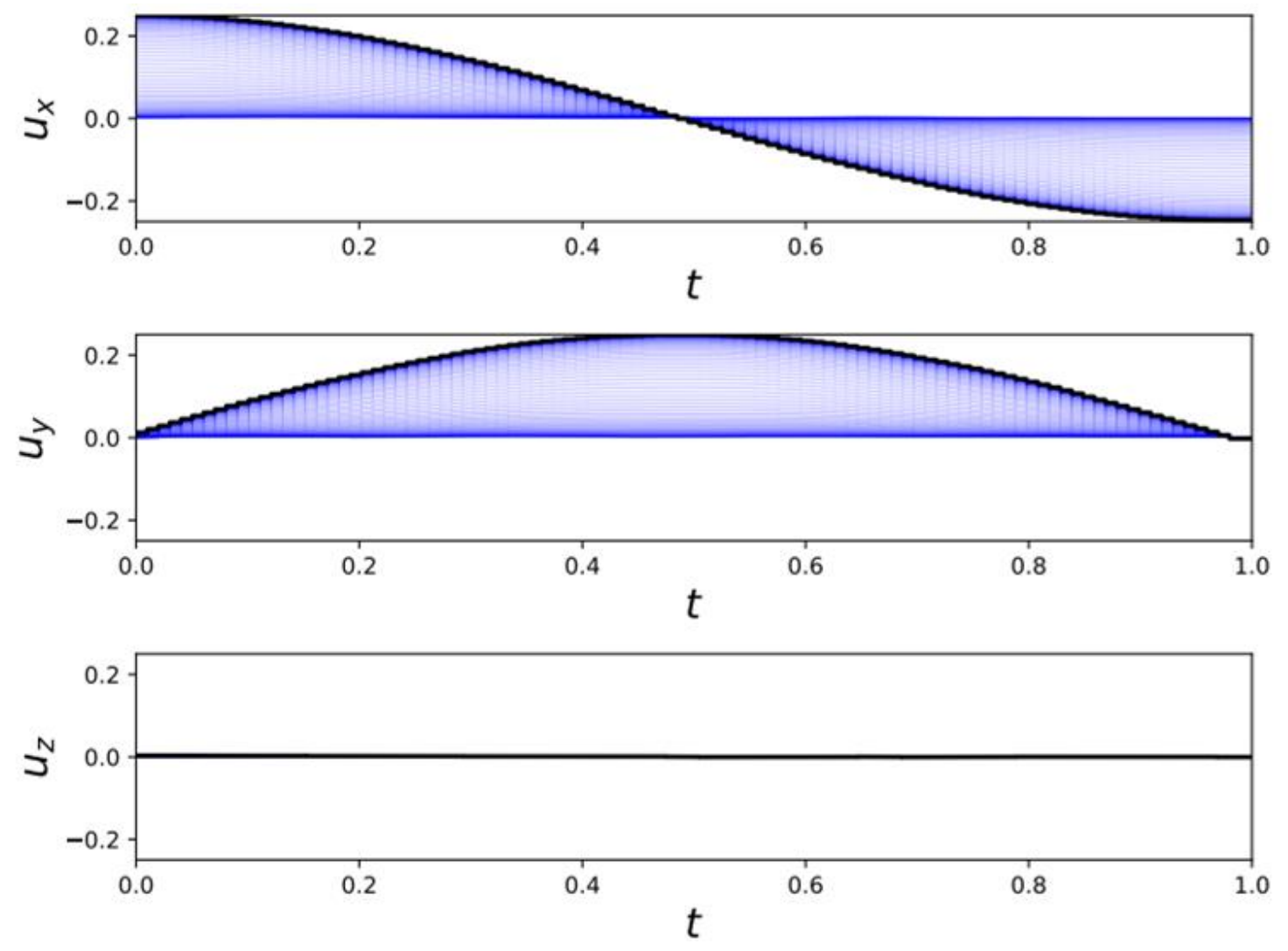
Single Qubit Unitaries

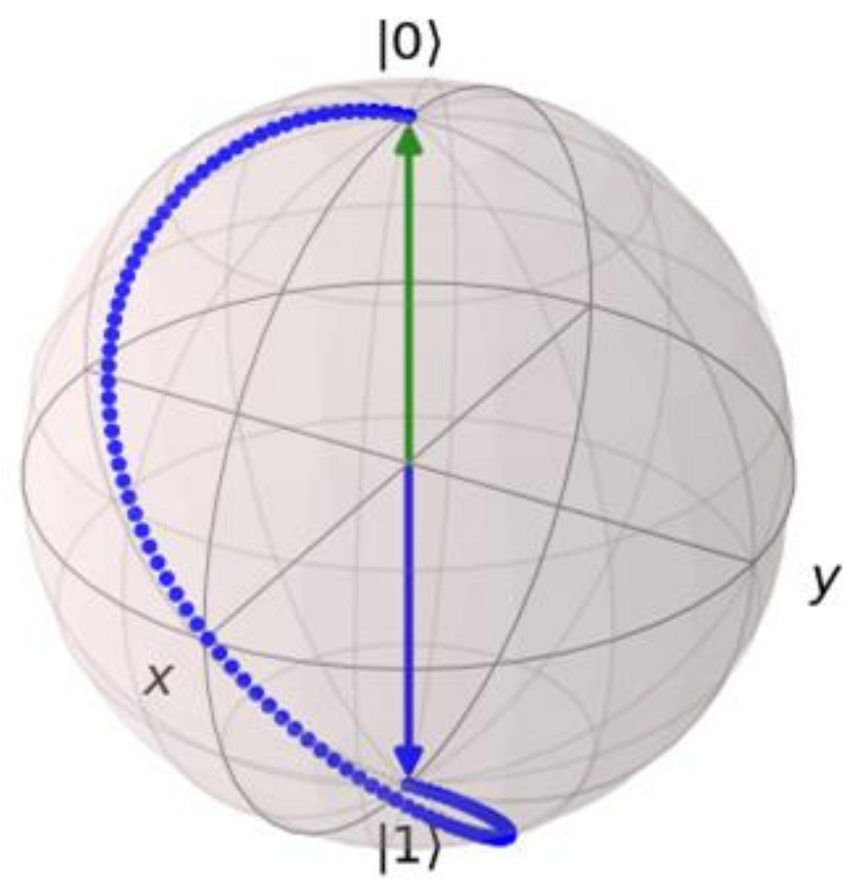
- To get familiar with GRAPE, we first attempted a R_Y rotation on a single qubit using python's QuTIP package
- Our drift hamiltonian is $H = \frac{0.1\pi\sigma_z}{2}$
- GRAPE was able to execute this transition with a fidelity of 0.999

$$RY = \begin{pmatrix} cos(\frac{\theta}{2}) & -sin(\frac{\theta}{2}) \\ sin(\frac{\theta}{2}) & cos(\frac{\theta}{2}) \end{pmatrix}$$

$$|\Psi_{initial}\rangle = |0\rangle$$

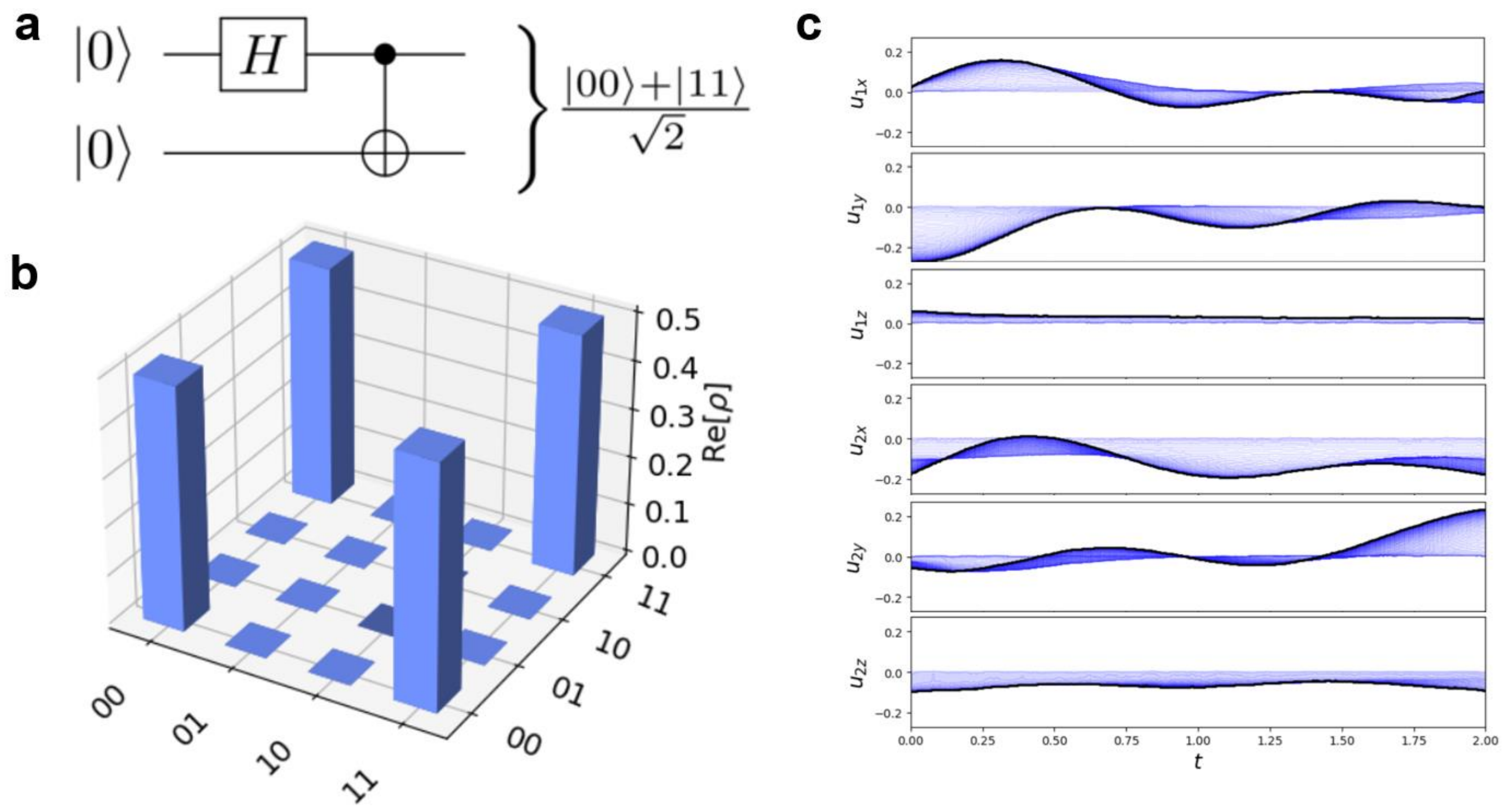
$$|\Psi_{final}\rangle = |1\rangle$$





Bell State Preparation

- As a demonstration of the GRAPE algorithm for a multi-qubit system, we calculate a sequence of single qubit control pulses which, in conjunction with a dipole-dipole coupling interaction between the qubits in the drift Hamiltonian, realizes a unitary matrix which prepares an entangled Bell state (**a**).
- The calculated unitary acting on |00⟩ produces a Bell state, as shown in (**b**). Amplitudes of the x, y and z components for each qubit of the applied control pulse are shown in (**c**).



NV Center Hamiltonian

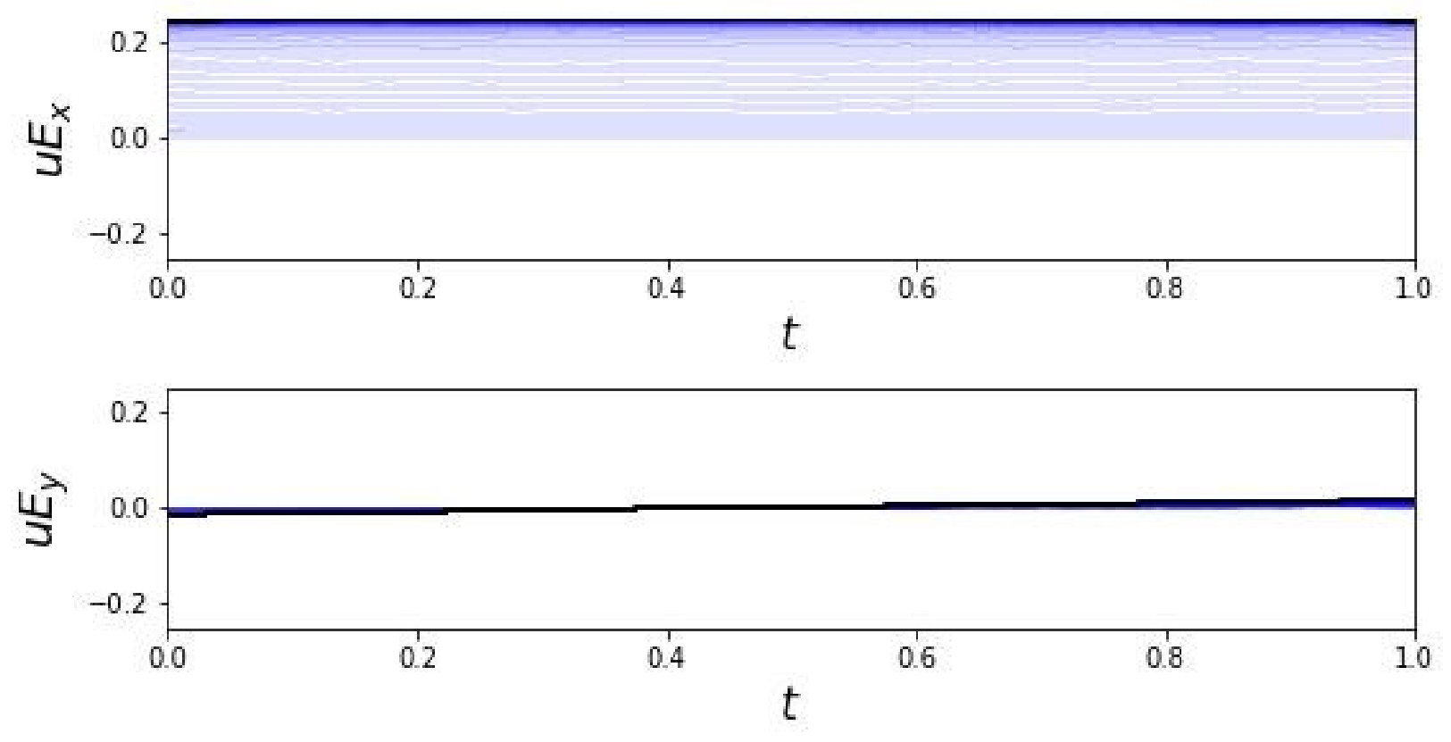
$$\hat{H} = \overbrace{\hbar D\left[\hat{S}_Z^2 - \frac{2}{3}\right] + \hbar E(\hat{S}_X^2 - \hat{S}_Y^2)}^{\text{zero-field term}} + \overbrace{\hbar\gamma_{nv}\vec{B}\cdot\hat{\vec{S}}}^{\text{magnetic interaction}} \overbrace{+\hbar\delta_{\parallel}\mathcal{E}_Z\left[\hat{S}_Z^2 - \frac{2}{3}\right] - \hbar\delta_{\perp}\left[\mathcal{E}_X(\hat{S}_X\hat{S}_Y + \hat{S}_Y\hat{S}_X) + \mathcal{E}_Y(\hat{S}_X^2 - \hat{S}_Y^2)\right]}^{\text{electric interaction}}$$

$$+\hbar\sum_{i=1}^{n}\left(\underbrace{\hat{\vec{S}}\mathcal{N}_i\hat{\vec{I}}_i}_{\text{hyperfine interactions}} + \underbrace{\gamma_i\vec{B}\cdot\hat{\vec{I}}_i}_{\text{nuclear Zeeman interactions}} + \underbrace{Q_i\hat{I}_{Z,i}^2}_{\text{nuclear quadrupole interactions}}\right).$$

Implementing the NV$^-$ in GRAPE

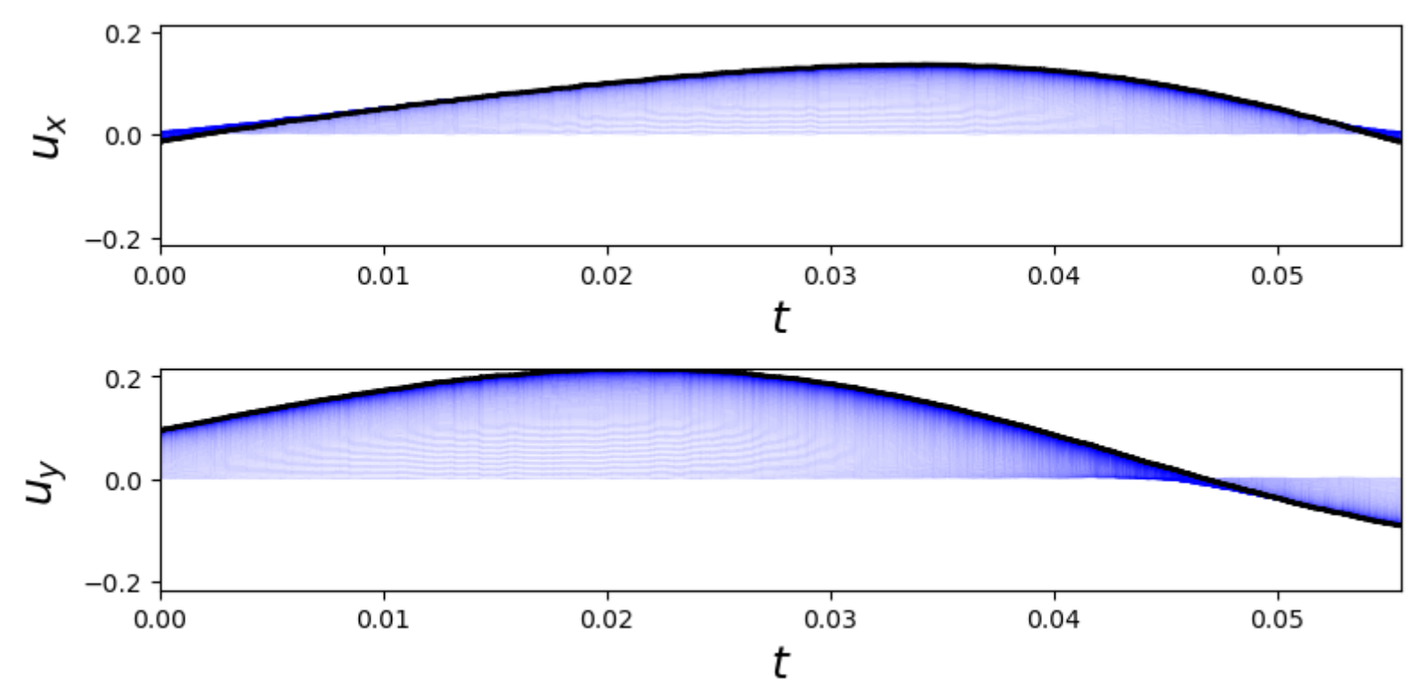
- We used GRAPE on the NV Hamiltonian to perform a R_X rotation on the electric qubit, with a fidelity of 0.999

$$|\Psi_i\rangle = \begin{pmatrix}1\\0\\0\\0\\0\\0\\0\\0\\0\end{pmatrix} \quad |\Psi_{if}\rangle = \begin{pmatrix}0.5\\0\\0\\-\frac{i}{\sqrt{2}}\\0\\0\\-0.5\\0\\0\end{pmatrix} \quad |\Psi_f\rangle = \begin{pmatrix}0.497 - i0.0492\\0\\0\\-0.0118 - i0.707\\0\\0\\-0.499 + 0.0173\\0\\0\end{pmatrix}$$



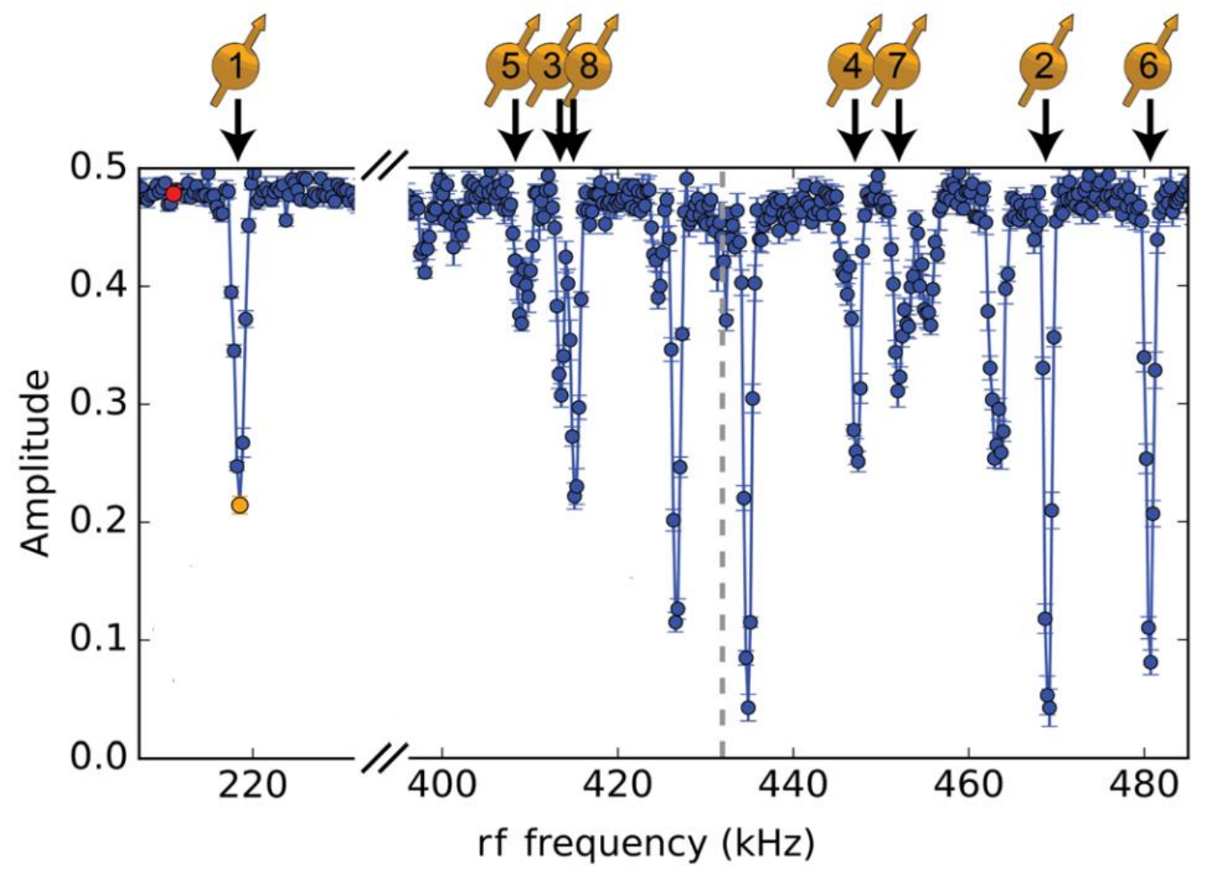
- To demonstrate physically what parameter would be varying, we can consider only the Zeeman splitting for the electron spin
- Assuming a static magnetic field perpendicular to the NV axis and a circularly polarized microwave field parallel to the NV-axis, we can perform the rotating wave approximation to get the following Hamiltonians.
- $H_{Zeeman} \approx \hbar\Delta\hat{s}_z + \Omega(t)(\hat{s}_x cos\phi(t) + \hat{s}_y sin\phi(t))$
- From here, the control and drift terms are identifiable as follows
- $H_{control,1} = \hat{s}_x \quad H_{control,2} = \hat{s}_y \quad H_{drift} = \Delta\hat{s}_z$
- Below is the GRAPE output for an R_X rotation on the electric qubit with fidelity of 0.999

$$|\Psi_i\rangle = \begin{pmatrix}1\\0\\0\\0\\0\\0\\0\\0\\0\end{pmatrix} \quad |\Psi_{if}\rangle = \begin{pmatrix}0\\0\\0\\-i\\0\\0\\0\\0\\0\end{pmatrix} \quad |\Psi_f\rangle = \begin{pmatrix}0\\0\\0\\0.2873 - i0.9579\\0\\0\\0\\0\\0\end{pmatrix}$$



^{13}C Dipole-Dipole Noise

- Spin-½ ^{13}C nucleii, which occur with a natural abundance of 1.1% in diamond, can couple to the NV$^-$ electron spin via dipole-dipole interactions.
- Though the existence of ^{13}C spins can be useful for building a multi-qubit register, the interaction terms can reduce the fidelity of NV$^-$ qubit gate operations
- We address this in GRAPE using a third 'noise' qubit. In practice, the ^{13}C couplings can be obtained via nuclear spin spectroscopy (figure).



Future Work, References, and Acknowledgments

- Developing a more sophisticated model for noise.
- Incorporating GRAPE rf pulse optimization into the experimental NV setup in the QT$^{(3)}$ lab.

1. Rembold, P. et al. Introduction to Quantum Optimal Control for Quantum Sensing with Nitrogen-Vacancy Centers in Diamond. AVS Quantum Sci. 2, 024701 (2020).
2. Bradley, C. E. et al. A Ten-Qubit Solid-State Spin Register with Quantum Memory up to One Minute. Phys. Rev. X 9, 031045 (2019).
3. Rondin, L. et al. Magnetometry with nitrogen-vacancy defects in diamond. Rep. Prog. Phys. 77, 056503 (2014).
4. Doherty, M. W. et al. The nitrogen-vacancy colour centre in diamond. Physics Reports 528, 1–45 (2013).

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