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# Nitrogen-Vacancy (NV) Centers in Diamond

# Magnetometry and Thermometry

Quantum Metrology Laboratory 1

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**Abstract**

**Nitrogen–vacancy** (NV) centers in diamond are atomic-scale defects whose electron spin can be read out optically at room temperature. By shining green light and sweeping a microwave frequency (optically detected magnetic resonance, ODMR), we observe dips in fluorescence at the NV spin transition. Magnetic fields shift these resonances via Zeeman effect, and a temperature difference shifts the zero-field splitting, so the same sensor can measure both field and temperature. Because NV centers point along four crystal axes, we can reconstruct the full 3D magnetic field.

## Contents

# 1 Theoretical Background

Nitrogen–vacancy (NV) centers in diamond are a paradigmatic example of a solid-state quantum system that can be used as a sensor for magnetic fields, temperature and other quantities. In this laboratory exercise you will use an ensemble of NV centers in a diamond sample to perform two basic but powerful types of measurements:

- **Magnetometry:** extracting the magnitude of an applied magnetic field from the Zeeman splitting of the NV spin levels.
- **Thermometry:** extracting temperature changes from shifts in the NV zero-field splitting.

The aim of this introduction is to provide a concise theoretical background for these experiments. We first review the structure and spin properties of the NV center, then introduce optically detected magnetic resonance (ODMR), and finally explain how the same physical principles lead to magnetometry and thermometry.

## 1.1 Quantum sensing with NV centers

Quantum sensing refers to the use of well-controlled quantum systems as probes of external fields and perturbations. A quantum system with discrete energy levels is extremely sensitive to its environment. Small changes in magnetic field, electric field, temperature or strain can shift transition frequencies or modify coherence times, and these changes can be read out with high precision.

NV centers in diamond are particularly attractive systems for sensing because they combine several practical advantages:

- They operate at room temperature and under ambient conditions.
- They are embedded in a robust solid-state host (diamond), which is chemically and mechanically stable.
- They can be initialized and read out optically with relatively simple optics (green laser excitation and red fluorescence detection).
- Their electron spin is sensitive to magnetic fields (via the Zeeman effect) and to temperature (via the temperature dependence of the zero-field splitting).

Depending on the experimental configuration, one can use a single NV center for nanoscale, spatially resolved sensing, or an ensemble of many NV centers for higher signal and wide-field sensing. In this lab we will work with an ensemble, focusing on the basic spectral signatures rather than on spatial resolution.

## 1.2 Structure and charge states of the NV center

Diamond is a wide-band-gap semiconductor with carbon atoms arranged in a tetrahedral ($sp^3$) lattice. An NV center is a point defect consisting of a substitutional nitrogen atom (replacing a carbon atom) adjacent to a lattice vacancy. This nitrogen–vacancy pair forms the NV defect. A representation of this structural layout can be found in Figure 1.

The NV center can exist in multiple charge states, the two most relevant being $NV^0$ and $NV^-$. The negatively charged state $NV^-$ is the one used for most sensing applications, because it possesses a spin-triplet ground state. Throughout this manual we will implicitly refer to $NV^-$ when we say "NV center".

Due to the symmetry of the diamond lattice, the NV axis can be oriented along four equivalent $\langle 111 \rangle$ crystallographic directions. In a bulk diamond sample, one typically has NV centers

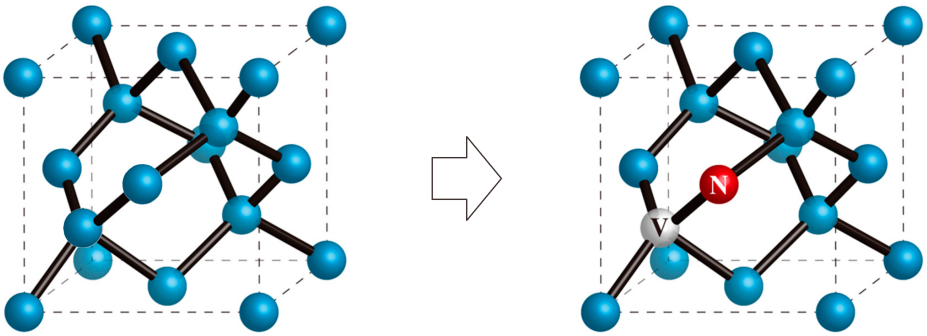


Figure 1: Pristine tetrahegonal diamond lattice (left), which through a substitutional nitrogen (red) and an adjacent vacancy (grey) gives rise to a Nitrogen Vacancy (NV) center. Adapted and modified from Figure 1 of S. Ishii et al, Quantum Beam Sci. 6(1), 2 2022.

in all four orientations. In an ensemble measurement, the observed spectrum is effectively an average over many NV centers, though in some situations particular orientations can be selectively addressed by choosing the direction of the applied magnetic field.

### 1.3 Spin triplet ground state and zero-field splitting

The ground electronic state of the $NV^-$ center is a spin triplet with total spin $S = 1$. In the absence of external fields, the three spin sublevels can be labeled by the projection quantum number $m_s \in \{0, \pm 1\}$, giving the states $|m_s = 0\rangle$ and $|m_s = \pm 1\rangle$.

Even when no magnetic field is applied, these three sublevels are not degenerate. Internal spin–spin interactions in the defect produce a zero-field splitting between $|0\rangle$ and $|\pm 1\rangle$, characterized by a parameter $D$. At room temperature, $D$ is approximately

$$D \approx 2.87 \text{ GHz}. \tag{1}$$

In energy-level diagrams, one typically draws the $|m_s = 0\rangle$ state lower in energy, and the $|m_s = \pm 1\rangle$ states elevated by an energy corresponding to the frequency $D$. Transitions between $|0\rangle$ and $|\pm 1\rangle$ can therefore be driven by microwaves at frequencies around 2.87 GHz.

At this stage it is useful to keep in mind that $D$ is not a fixed fundamental constant: it depends on temperature and on local strain in the diamond. This temperature dependence is precisely what enables NV-based thermometry.

### 1.4 Optical pumping and spin-dependent fluorescence

The NV center offers a convenient way to initialize and read out its spin state using optical excitation and fluorescence detection. Under green laser excitation (for example, a 532 nm laser), the NV center is excited from its ground-state triplet to an excited-state triplet. From there, it can decay back to the ground state by emitting red fluorescence photons (typically in the 650–800 nm range).

In addition to this radiative cycle, there exists a non-radiative pathway via intersystem crossing through intermediate singlet states. Crucially, the probability of decaying through this pathway depends on the spin state: the $|m_s = \pm 1\rangle$ states have a higher probability to undergo intersystem crossing than the $|m_s = 0\rangle$ state. The singlet manifold predominantly relaxes back to the ground state in the $|0\rangle$ sublevel.

The combined effect of repeated optical excitation and decay is twofold:

- The NV center is **optically polarized** into the $|m_s = 0\rangle$ state, a process often called spin initialization.

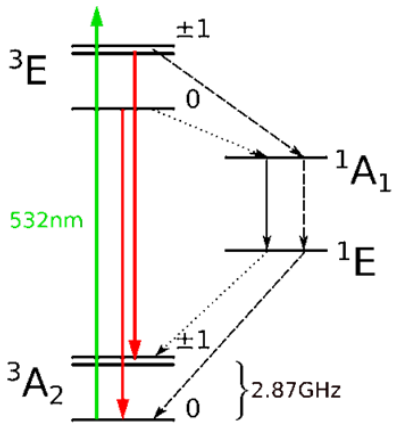


Figure 2: Energy level diagram of the $NV^-$ center system, including both ground state and excited triplet states and the intersystem crossing pathways through the intermediate singlet states (Adapted from https://www.qolah.org/research/nv_v2/nv_v2.html)

- The average fluorescence intensity is **spin-dependent**: the NV is brighter when it is in $|0\rangle$ and dimmer when it is in $|\pm1\rangle$.

This spin dependence of the fluorescence is what allows us to read out the spin state: by monitoring the fluorescence intensity while driving microwave transitions between the spin sublevels, we can infer which transitions are resonant.

### 1.5 Ground-state spin Hamiltonian and Zeeman effect

At low energies, the NV center ground-state spin triplet can be described by an effective spin Hamiltonian. In its simplest form, neglecting strain and hyperfine interactions, this Hamiltonian reads

$$\hat{H} = D\hat{S}_z^2 + \gamma_e \vec{B} \cdot \hat{\vec{S}}, \tag{2}$$

where

- $D$ is the zero-field splitting parameter introduced above,
- $\hat{\vec{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ is the spin-1 operator,
- $\vec{B}$ is the external magnetic field, and
- $\gamma_e$ is the electron gyromagnetic ratio (approximately $28\,\mathrm{GHz\,T^{-1}}$).

The first term, $D\hat{S}_z^2$, lifts the degeneracy between $|0\rangle$ and $|\pm1\rangle$ even when $\vec{B} = 0$. The second term describes the Zeeman interaction with an external magnetic field. If the magnetic field has a component $B_\parallel$ along the NV axis (chosen as the $z$-axis in this effective model), then, to first order, the energies of $|m_s = \pm1\rangle$ shift linearly with $B_\parallel$, while $|m_s = 0\rangle$ remains essentially unchanged.

In terms of transition frequencies between $|0\rangle$ and $|\pm1\rangle$, this gives approximately

$$f_\pm \approx D \pm \gamma_e B_\parallel, \tag{3}$$

so that the splitting between the two resonances is

$$\Delta f = f_+ - f_- \approx 2\gamma_e B_\parallel. \tag{4}$$

This simple relation between the frequency splitting and the magnetic field component along the NV axis is the basis of NV magnetometry in this lab.

### 1.6 Optically detected magnetic resonance (ODMR)

Optically detected magnetic resonance (ODMR) is the central experimental technique used in this lab. It combines continuous optical excitation and spin readout with a microwave drive of the spin transitions.

The basic ODMR protocol is as follows:

1. Illuminate the diamond with green laser light to continuously excite the NV centers and polarize them into the $|m_s = 0\rangle$ state.
2. Apply microwaves with frequency $f$ in the GHz range to drive transitions between $|0\rangle$ and $|\pm 1\rangle$.
3. Slowly sweep $f$ across the expected resonance region (around 2.87 GHz) while monitoring the red fluorescence intensity.

Whenever the microwave frequency is resonant with one of the spin transitions, population is transferred from the brighter $|0\rangle$ state to the darker $|\pm 1\rangle$ states. This leads to a small dip in the measured fluorescence intensity. Plotting fluorescence as a function of microwave frequency therefore yields a spectrum with one or more dips at the resonance frequencies. This is the ODMR spectrum.

In an ensemble experiment, the ODMR contrast (depth of the dips relative to the background fluorescence) is typically a few percent. To accurately extract the resonance frequencies, one often fits the dips with a suitable line shape, such as a Lorentzian or Gaussian profile. In this lab you will use such fits to determine the positions and splittings of the ODMR resonances.

### 1.7 NV-based magnetometry

From the perspective of magnetometry, the crucial point is that the ODMR resonance frequencies depend on the magnetic field via the Zeeman effect. If the field is oriented approximately along the NV axis, the two transition frequencies $f_\pm$ follow Eq. (3). The splitting between them, Eq. (4), is then directly proportional to the field component $B_\parallel$.

In practice, the magnetometry procedure in this lab proceeds as follows:

- Record an ODMR spectrum with no external magnet (or with a known reference configuration) to identify the baseline resonance around $D$.
- Introduce a magnet near the sample to apply a finite magnetic field and record a new ODMR spectrum. The single resonance is now expected to split into two dips corresponding to $f_+$ and $f_-$.
- Fit the spectrum to extract the resonance frequencies and compute the splitting $\Delta f$.
- Use Eq. (4) to estimate the magnetic field component $B_\parallel$ at the NV centers.

The sensitivity of an NV-based magnetometer depends on several factors, including:

- The linewidth of the ODMR transitions (related to the spin dephasing time $T_2$ ),
- the fluorescence contrast between $|0\rangle$ and $|\pm 1\rangle$, and
- the photon detection rate (which sets the shot-noise level).

In this setup, we will not optimize these quantities for ultimate sensitivity, but they still play a role in determining how precisely you can locate the resonance positions and thus estimate the magnetic field.

### 1.8 NV-based thermometry

In addition to magnetic field, the zero-field splitting parameter $D$ is also sensitive to temperature. As the temperature changes, thermal expansion of the diamond lattice and electron–phonon interactions modify the spin–spin interaction that sets $D$. Around room temperature, this dependence is approximately linear, and can be written as

$$D(T) \approx D_0 + k_T \left(T - T_0\right), \tag{5}$$

where $D_0$ is the value of $D$ at some reference temperature $T_0$, and $k_T$ is a temperature coefficient (typically on the order of $\sim 10^5$–$10^6$ Hz/K, depending on the sample and conditions).

If the magnetic field is held constant, a change in temperature $\Delta T$ leads to a shift in the resonance frequency

$$\Delta D = D(T) - D(T_0) \approx k_T \Delta T, \tag{6}$$

so that

$$\Delta T \approx \frac{\Delta D}{k_T}. \tag{7}$$

Thus, by measuring how the ODMR resonance frequency changes with temperature, and knowing (or calibrating) $k_T$, one can use NV centers as local thermometers.

In this lab, the basic thermometry procedure will be:

- Fix the magnetic field configuration (or minimize stray fields) so that field-induced shifts are constant.
- Vary the temperature of the diamond sample in controlled steps using a heater or Peltier element, and measure the sample temperature with an external sensor.
- At each temperature, record an ODMR spectrum and extract the resonance frequency (or effective $D$).
- Plot the resonance frequency as a function of temperature and fit a straight line to extract an experimental value of $k_T$.

Once $k_T$ is known, any subsequent shift in the measured resonance frequency can be converted into an estimated temperature change, within the limits set by noise, temperature stability and possible cross-sensitivities.

It is important to note that both magnetic field and temperature can affect the resonance frequencies. In more advanced protocols, one can use multiple transitions, different NV orientations or specific pulse sequences to disentangle magnetic and thermal effects. In this introductory experiment, we will treat the magnetic field as fixed during thermometry runs and attribute observed frequency shifts primarily to temperature changes.

## 2 Experimental Setup and Preparation

### 2.1 Setup Description

The setup is controlled from the computers present in the laboratory. They already have the necessary drivers installed. The first step is to ensure the computers are connected via USB to the E-QS-CU100 Quantum Sensing Control Unit, henceforth called "driver" (see Figure 3), and connect it to its power supply. On the front panel of the driver, one can see a Power button, then a connector for the sensorhead or optical setup marked as "Sensor" and finally two extension ports marked as "EXT1" and "EXT2".


Figure 3: Close-up image of the E-QS-CU100 Quantum Sensing Control Unit.

In the back there is an Ethernet port, a USB port and a Power supply connection rated at 12 VDC, with a maximum power of 60 W. The device can then be turned on by pressing the power button, which should light blue once it is connected. The manual for this device can be found inside the USB-stick named AQ-EDU, which should be attached to the control computer.

One can connect to the driver two different NV center measurement setups via the Sensor port. The first one is an optical table setup (see Figure 4), with labels. Note there is a 532 nm laser being focused onto the diamond sample, which is an NV center ensemble, and then a photodetector to collect the fluorescence.

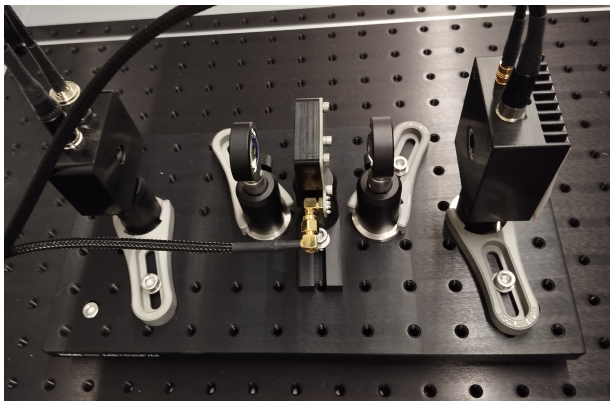

Figure 4: Optical table setup for NV center magnetometry with labels.

The second possible NV center sensor setup is a sensor head that has all the elements of the optical board integrated, such that one can make other more advanced experiments. This sensor head can be seen in Figure 5, and the schematics of its inner workings are in Figure 6.

The optical board setup will be used to perform an ODMR in a first, more pedagogical way, such that we can actually see how the setup is working. However, in order to be able to make a controlled magnetometry and thermometry, we will use the sensor head, since it is significantly more compact (the diamond sample is at the tip of the sensor head) and there is an adapted setup with a Helmholtz coil and a build-in temperature probe, which can be seen in Figure 7 that will be used for the 3D vector magnetometry and thermometry experiments.

The Helmholtz coil will allow full control over the three components of the magnetic field, which we can then reconstruct on the respective applet on the GUI. Please note that, while

Figure 5: Sensor head for NV center sensing.

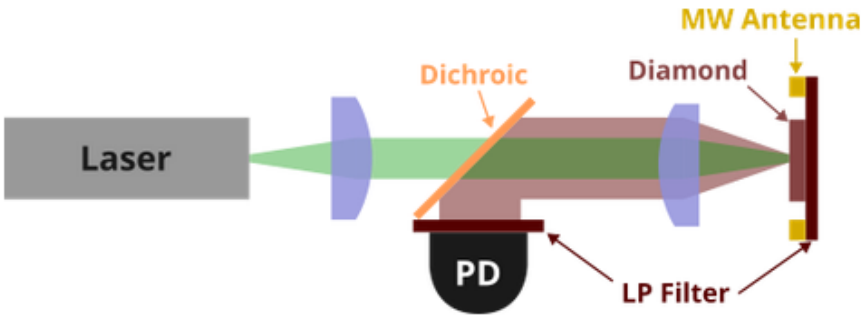


Figure 6: Schematic representation of the NV ensemble sensor head. The optical setup is a board version of this setup, but with the fluorescence being collected after the diamond sample instead (and therefore no dichroic mirror is necessary before the photodetector).

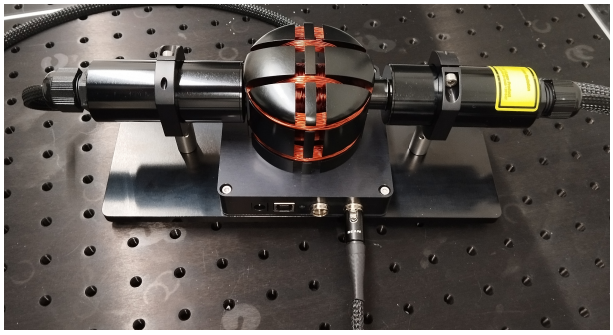

Figure 7: Vector magnetometry and thermometry setup.

both the Helmholtz coil and the temperature probe are mounted simultaneously, we will be performing the experiments using only one of them at the same time. This is made to ensure that we can cleanly retrieve either the magnetic field of temperature shifts independentely, although one could, in principle, come up with a protocol to measure both simultaneously, and there are many such techniques.

### 2.2 Launching an Experiment

Inside the AQ-EDU stick, one can also find, inside a folder named "server", the AQConnection-Server.exe executable. This can be run without intallation and will access the device and open a new tab in the web browser with a graphical user interface (GUI) showing the available devices

(see Figure 8).

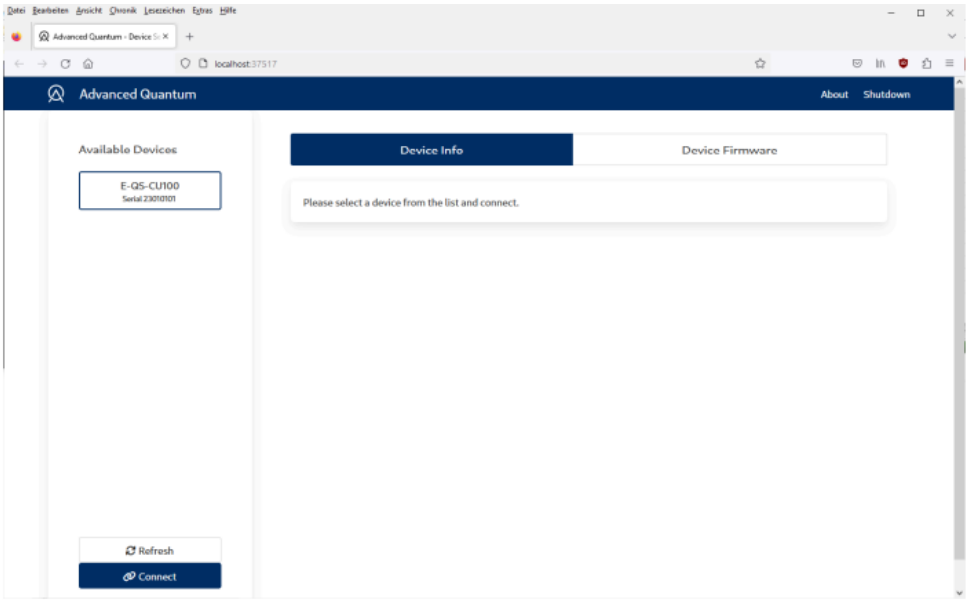


Figure 8: Snapshot of the control unit's GUI startup page.

Depending on which experiment we want to run, we will see a different available device. Upon selecting the desired one, one presses Connect and another tab will pop up, this one with the main control tab, from here, we are able to run the experiments.

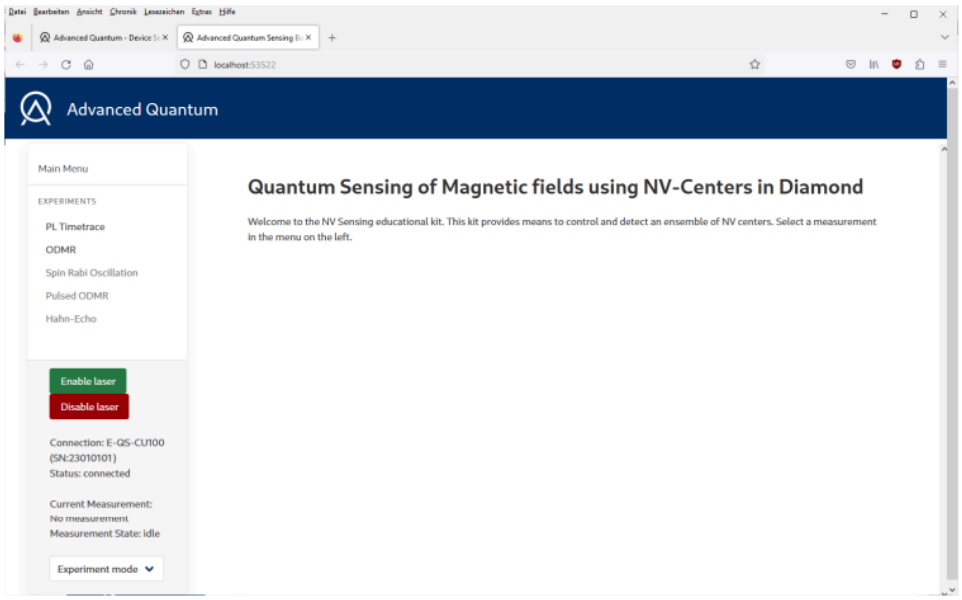


Figure 9: Control unit's GUI main page.

On the bottom, a drop-down menu allows the choice between course mode and experiment mode. We should switch to course mode. There are, on the left side, various pages that one can open, namely Classes (which contain a series of pages with information about color centers, the setup itself and spin physics) and also, under "Quantum Sensing", the applets for running each of the experiments.

# 3 Experiment A: NV Magnetometry

To measure the Zeeman splitting of the NV center ODMR resonances as a function of an external magnetic field and extract the magnetic field magnitude from the resonance frequencies. This will be done in two ways: firstly using the optical setup (to get familiar with the working principles of the ODMR) and then using the compact probe inside the magnetometer for 3D vector magnetometry, for a more serious and controlled ODMR.

## 3.1 Experiment A.1: Simple Magnetometry

### 3.1.1 Experimental Procedure

- Dim the lights of the laboratory.
- Connect the optical setup to the Sensor port of the driver and run the GUI in Course mode. Open the ODMR Magnetometry applet.
- Define the laser power. You can start with a fairly low power (say $\sim 20\%$) and increase it to see the effect this has on the data.
- Define the microwave power. You can start with the default one (0 dBm) and change it to see the effect it has on the plot.
- Define the center frequency around the zero-field splitting and define a frequency span that makes sense considering the kind of magnetic fields you are expecting to see (e.g. background, small magnet, etc.).
- Define the sweep such that you get a clean plot (enough accumulations) within a reasonable time.
- Run a first measurement to characterize the intrinsic splitting due to the environment and the crystal. This defines an offset for the next measurements using this setup.
- There is a small Neodymium magnet in the lab. By placing it on the base of the optical holder that has the diamond sample (approximately along the vertical axis), and by running a new experiment you should be able to see an increase of the splitting.
- Calculate the intensity of the magnetic field (assuming it is along the NV axis) induced by the magnet on the magnet.

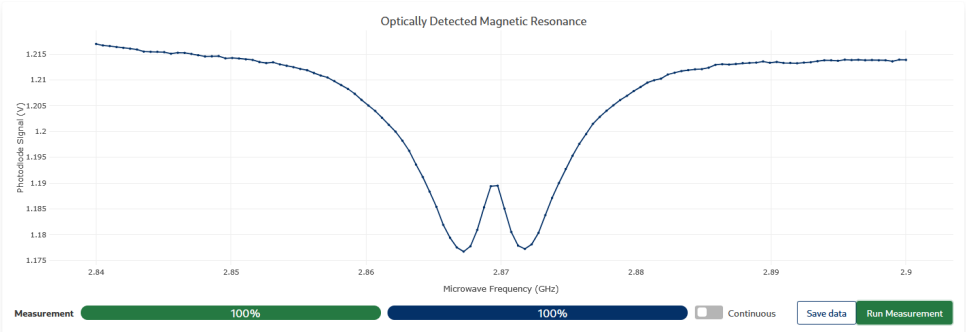


Figure 10: Example ODMR using the optical setup.

### 3.1.2 Conceptual Questions

- How does the quality of the signal change with the intensity of the laser?
- How does the ODMR contrast change with microwave power?
- What limits the sensitivity of the magnetometer in this setup?

## 3.2 Experiment A.2: Vector Magnetometry

### 3.2.1 Experimental Procedure

- Connect the sensor head to the driver and link the external connector of the Helmhotz coil to the
- Dim the lights of the laboratory.
- Connect the optical setup to the Sensor port of the driver and run the GUI in Course mode. Open the Vector Field Decomposition applet.
- Define the laser power, microwave power, center frequency and sweep parameters optimally, based on what you gathered from the previous experiment.
- Run measurements for different magnetic field excitations to get familiar with the framework, namely along the three axis. Infer which axis of the coil corresponds approximately to the NV axis.
- Find the constant of proportionality between magnetic field and current applied in the coil. This can be done by applying different magnetic fields along the axis you identified as the NV one (i.e., the splitting is approximately linear) and obtaining a correspondence between current and magnetic field. We assume this is the same for the three axes, which is a liberal assumption since at the center of a single-axis Helmholtz coil this is

$$\frac{B}{I} = \left(\frac{4}{5}\right)^{3/2} \frac{\mu_0 n}{R}, \tag{8}$$

  for a pair of coils of radius R, n turns and $\mu_0$ the permeability of free space - we assume the coil is well calibrated and was designed in order to give an equivalent relation between current and magnetic field in each axis.
- Let's now allow the magnetic field to be arbitrary and derive the full Hamiltonian with zero-field splitting and Zeeman effect. Reparametrize this to parallel and perpendicular components using $B_\perp = \sqrt{B_x^2 + B_y^2}$ and $B_z = B_z$, and rotating the coordinate system around $z$ so that the new rotated frame is $(B_x, B_y, B_z) \to (B_\perp, 0, B_z)$.
- This corresponds to the full Hamiltonian for a single NV center. Run a sweep, say $(I_x, I_y, I_z) = (200, 200, 200)$ mA. How many big dips do we see and how many did we expect based on the dimension of the Hamiltonian? Why is there a discrepancy?
- Let's now introduce the fact that there are four NV axis. How many dips do we expect? How many do we observe?
- Discuss the physical significance of the smaller dips, namely what factors have not been accounted for but become relevant for larger magnetic fields and arbitrary directions.

# 4 Experiment B: NV Thermometry

## 4.1 Objective

To observe temperature-induced shifts in the NV center ODMR resonance and use them to estimate local temperature changes.

## 4.2 Experimental Procedure

- Connect the temperature sensor/heater to the driver.
- Remove the Helmholtz coil from the stand.
- Place the temperature sensor touching the end of the sensor head.
- Define the laser power, microwave power, center frequency and sweep parameters optimally, based on what you gathered from the previous experiment.
- Define a reference temperature and obtain the respective zero-field splitting position.
- Change the temperature around that reference and perform various ODMR measurements. This will allow a plot of D as a function of T.
- Extract the temperature coefficient $k_T$ from a linear fit and find the associated uncertainty. Discuss the physical significance of the linear fit coefficients.
- Estimate the smallest resolvable temperature change given your frequency resolution.

## 4.3 Discussion Points

- Compare your measured $k_T$ to literature values.
- Discuss possible cross-sensitivity between magnetic field and temperature.
- (Conceptual, optional) Can you conceive a protocol that separates magnetic and thermal effects?

## 5 Laboratory Report

After completing the laboratory work, the students should elaborate a concise group report regarding the setup, results, discussion and conclusions. A proposed minimal structure is as follows, but there is freedom in the structure, content and extent of the discussion. The report should also include the discussion points and plots already obtained and described in the experiment description, as well as some reflection on the guiding questions.

1. **Introduction**
   - Briefly explain what NV centers are and why they can be used as quantum sensors.
   - Shortly describe the physics behind nitrogen vacancy centers, the structure of their energy levels and the the ODMR protocol.
   - State the goals of the magnetometry and thermometry experiments.
2. **Experimental Methods**
   - Describe the setups (including, for instance, a diagram or photo).
   - Summarize the measurement procedures for both simple and vector magnetometry and thermometry.
3. **Results**
   - Present representative ODMR spectra (figures).
   - Show processed data (e.g. resonance frequency vs. field/temperature).
   - Include tables with fitted parameters and uncertainties.
4. **Analysis and Discussion**
   - Discuss how the resonance frequency depends on magnetic field and temperature.
   - Comment on the sensitivity and main sources of noise/uncertainty.
5. **Conclusion**
   - Summarize what you learned about NV-based magnetometry and thermometry.
   - Suggest one improvement to the experimental setup or protocol.