Title of my Dissertation

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August XX, 2024

MSc in Theoretical Physics

The University of Edinburgh

2023

Abstract

This is where you summarise the contents of your dissertation. It should be at least 100 words, but not more than 250 words.

Declaration

I declare that this dissertation was composed entirely by myself.

Personal Statement

You **must** *include a Personal Statement in your dissertation. This should describe what you did during the project, and when you did it. Give an account of problems you faced and how you attempted to overcome them. The examples below are based on personal statements from MSc and MPhys projects in previous years, with (mostly-obvious) changes to make them anonymous.*

Acknowledgements

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Chapter 1

Introduction

The field of spectroscopy studies the way atoms and molecules interact with and exchange energy with a wider physical system - specifically through electromagnetic radiation. The electric field interacts with with the electric dipole moment and the magnetic field interacts with a magnetic dipole moment. Magnetic resonance spectroscopy focusses specifically on the interaction between the **B** field with magnetic moments which exist in a given material. This can be broken into two distinct fields:

Nuclear Magnetic Resonance (NMR) which studies the interaction with nuclear magnetic moments.

Electron Paramagnetic Resonance (EPR) which studies the interaction with magnetic moments of electrons.

Using Planck's relationship $E = h\nu$ and $c = \lambda\nu$ we may characterise the electromagnetic radiation by its energy which is, to a constant, equivalent to the frequency or the wavelength. EPR is observed in systems where the magnetic dipole of the electron is influences by an applied, oscillating magnetic field forcing transitions between electron energy levels. In general the measurable difference in energy levels for which the transition occurs is caused by an external magnetic field via the Zeeman effect. Some systems also exhibit energy level splitting in the absence of an applied external magnetic field so called zero field splitting.

EPR is thus a tool to manipulate electron spins in solid state materials. The transition between energy levels is quantised thus the discrete amount of energy which is lost by the system is transferred into a photon or charge state which may be detected optically or electrically [1].

A particularly successful technique is Optically Detected Magnetic Resonance (ODMR) which uses an applied microwave frequency, an oscillating magnetic field with energy quanta equivalent to the transitions between Zeeman sub levels, to drive the repopulation of those Zeeman sub levels following a spin-dependent optical transition. In essence this boosts the sensitivity since the microwave driven repopulation induces a change in photoluminescence with a much higher and thus much more readily detectable energy. The techniques of ODMR are so effective that even a single electron spin may be detected this way [2].

Spintronics, a portmantau of **spin** and elec**tronics** is a technology which exploits the characteristics of spin akin to how charge is manipulated in electronics. Fundamentally, the smallest stable magnetic moment available in nature is generated by the spin of a single electron. If efficient read-out can be achieved, the sensitivity of the electron magnetic dipole cannot be matched. Careful construction of an appropriate system, or identification of a system with appropriate characteristics allows for the initialisation, manipulation and read-out of EPR from which we may infer the physical properties of the environment surrounding the system.

The properties of nitrogen-vacancy (NV) colour centres in diamond have catalysed major development in the field. The NV and ODMR have enabled the manipulation of spin states in single, atomic-sized centres at room temperature despite spin polariation being a primarily thermodynamic effect . This is possible since optical excitation of the energy levels decay faster via a spin-preserving transition, leading to an inverse population of spin sublevels in its ground state when the system is irradiated consistently for several excitation/decay cycles. Other structures with similar unique quantum properties are being identified. Specifically, Silicon carbide (SiC) is a promising candidate. A major benefit of SiC is the existence of various polytypes, which each exhibit unique spin colour centre properties. Furthermore, even within a single polytype, these centres can occupy distinct and non-equivalent lattice positions. The existence of these colour centres with similar properties but different energy quanta allows for selection of a specific defect with parameters suitable for the problem at hand.

need a reference for the thermodynamic comment

EPR can be approached by two different methods:

Consider writing a paragraph on ENDOR - only if relevant later in the project.

Continuous Wave the magnitude of the static magnetic field (B_0) is swept, while the amplitude of the driving field B_1 is constant with time.

Pulsed a time-dependent driving pulse B_1 is applied in addition to a static magnetic field B_0.

Need to write a section on using Pulsed EPR to measure relaxation timescales.

This work looks to explore how the physical characteristics which influence the Hamiltonian, thus the energy, of the electron spin may be inferred by measuring the effects of those characteristics on EPR of the specific system. Further, it will look to explore whether the compound effect of multiple influences may be disentangled and distinguished simultaneously.

Chapter 2

Background Theory

2.1 Magnetism

2.1.1 Magnetic Dipole

Where charge (**E**-field) has an intuitive elementary source unit of a point charge (or monopole) which may be positively or negatively charged. Conversely the elementary source unit of magnetism (**B**-field) is the magnetic dipole.

Classically, the magnetic dipole may be modelled as a closed loop that carries an electric current. Its magnetic dipole moment, $\vec{\mu}$, is defined as the vector which points out of the plane of the current loop,

$$\vec{\mu} = IS\vec{n} \tag{2.1}$$

where I is the current in the loop and S is the surface area enclosed by the loop.

The magnetic dipole produces a magnetic field $\vec{B}$, which for points a large distance from the dipole may be calculated as :

Type up derivation from David Tong notes

$$\vec{B} = \frac{\mu_0}{4\pi}\frac{1}{r^3}\left[\frac{3(\vec{\mu}\cdot\vec{r})\cdot\vec{r}}{r^2} - \vec{\mu}\right]$$

The symmetry of the field enables us to, without any loss of generality, consider the direction of the dipole the z-axis. Then, defining x, y as usual by $r\cos\theta$ and $r\sin\theta$ respectively. We may then consider magnetic field in two separate components, parallel (B_z) and perpendicular (B_x, B_y):

$$B_{\parallel} = \frac{\mu_0}{r^3}(3\cos^2\theta - 1), \quad B_{\perp} = \frac{3\mu_0}{r^3}\cos\theta\sin\theta.$$

Then, we may use the Pythagorean principle to determine the overall magnitude B as

$$B = \sqrt{B_{\parallel}^2 + B_{\perp}^2}.$$

2.1.2 Gyromagnetic Ratio

Classical Derivation

The current in equation 2.1 is proportional to the angular momentum of the charge. That is, the dipole moment is always associated with an angular momentum $\vec{G} = \vec{r} \times \vec{p}$ with $\vec{r}$ the radius and $\vec{p}$ the momentum.

Dividing the magnetic dipole moment by the angular momentum we find the **gyromagnetic ratio**.

$$\gamma = \frac{\vec{\mu}}{\vec{G}}. \tag{2.2}$$

Without loss of generality we may consider the most simple case which is where the magnetic dipole moment is parallel (or anti-parallel) to the angular momentum. Then we may consider the absolute values for the dipole moment and the angular momentum:

$$\mu = IS, \quad I = \underbrace{\frac{q}{2\pi R}}_{\rho \text{ (charge density)}} v, \quad S = \pi R^2 \tag{2.3}$$

We substitute I and S to find

$$\mu = \frac{qvR}{2} \tag{2.4}$$

and further, we equate the angular momentum vector, using the model of a planar loop to

$$G = m_q v R \tag{2.5}$$

leaving

$$\gamma = \frac{q}{2m_q}. \tag{2.6}$$

We finally consider that we may represent the, currently unknown, charge and mass as a sum of electron charges and masses. We therefore find that the gyromagnetic ratio of the electron depends only on constants

$$\gamma = \frac{q}{2m_q} = \frac{\cancel{N}e}{2\cancel{N}m_e} \implies \gamma = \frac{e}{2m_e}. \tag{2.7}$$

[3]

Extending to Quantum Mechanics

Since the gyromagnetic ratio was calculated considering the motion of dipole in a loop, we may extend this to an electron in an orbit within the atom. The fundamental change required to extend the model to quantum mechanics is the treatment of angular momentum which should now be quantized. Thus, we replace our classical approximation of $\vec{G} = \vec{r} \times \vec{p}$ with the equation for the eigenvalues of the quantum mechanical representation of orbital angular momentum:

$$\hat{G} = \hbar \hat{J} \tag{2.8}$$

where $\hat{J}$ is the operator of the orbital angular momentum (quantum number of orbital momentum).

2.1.3 Electron Magnetic Moment

[4]

Chapter 3

To Sort

3.1 Spin

The magnetic moment of elementary particles is called spin.

3.2 Defect Orientation

Colour centres or defects in general are part of the crystal lattice and thus have an associated orientation and direction within the lattice. This allows the definition of a **defect axis**. For example, in diamond the NV axis is defined as the vector from the vacancy towards the Nitrogen atom when the vacancy is taken as the origin of your co-ordinate system.

In a tetragonal crystal, due to symmetry there are four possible orientations of a defect within the lattice: 111, $1\overline{1}\overline{1}$, $\overline{1}1\overline{1}$ and $\overline{1}\overline{1}1$ directions.

3.3 Miller Indices

The notation for defect orientation above is known as a Miller Index, and we consider the 111 direction to be aligned with the defect axis.

This means that if we know the orientation of our crystal then we can establish the orientations of the defect axis inside. For example, using a crystal for which all surfaces belong to the {001} lattice planes, each surface normal is aligned with a Cartesian axis. Thus, by fixing the crystal in place, there remain just **four** possible angles which a defect axis can have with respect to the crystal surface.

Calculating the scalar product of any of the surface planar directions in the family of {001} and the four possible orientations of the defect within the lattice we find $\cos\theta = \pm 0.6$. Then, considering the physical solutions (from $0, 2\pi$) gives four possible angles that the (directed) defect axis may make with the surface of the crystal: 53.13°, 306.87°, 126.9° and 233.13° (0.927, 5.355, 2.214 and 4.069 radians respectively).

3.4 Lattice Symmetry

Tetragonal lattice has the

3.5 Linear Combination of Atomic Orbitals

3.6 Quantum Sensing

Quantum sensing involves using a qubit system acting as a quantum sensor that interacts with an external variable of interest, such as a magnetic field, electric field, strain or acoustic wave, or temperature [5].

Quantum sensors have a higher sensitivity within a nanoscale or microscale sampling volume compared to a fully classical counterpart which would require higher field densities or higher volume interrogation to be effective.

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3.6.1 DiVincenzo Criteria

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3.6.2 Crystal Defects

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Quantisation

Polarisation

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Coherent Manipulation

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Efficient Readout

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3.6.3 Coherence

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Spin Relaxation

Dephasing

Hahn Echo

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Example: NV Diamond

3.6.4 Sensitivity

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3.6.5 ODMR

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3.6.6 Multimodal Sensors

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3.7 Silicon Carbide

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3.7.1 Production of SiC

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3.7.2 Colour Defects in SiC

Electronic Structure

Charge State

Spin System

3.7.3 Wider Scientific Context

[65]

Chapter 4

Task

4.1 Brief

I think, as a start can go through section 3.2.4 in the attached PhD thesis? In particular check in details how to diagonalise the NV centre spin S=1 Hamiltonian to get Eq. 3.31? You could also do some python simulations to plot how the spin levels (i.e. the eigenvalues of the spin Hamiltonian) change with applied magnetic field.

Once we've learned this, we can apply it to other spin defects in SiC.

4.2 Work

4.2.1 Concepts and Nomenclature

Spin-Spin Interactions

Zeeman Splitting

Hyperfine Interaction

4.2.2 System Hamiltonian

The ground state of the NV^- spin system in diamond is a triplet state, thus a $S = 1$ system.

The corresponding Hamiltonian, which it seems can be generalised to an electron spin system of a defect, can be expressed as:

$$H_{\mathrm{NV}} = H_{\mathrm{D}} + H_{\mathrm{Zeeman}} + H_{\mathrm{HF}} \tag{4.1}$$

Here the labels D, Z and HF describe the electron spin-spin interactions, the Zeeman interaction with an external magnetic field and the hyperfine interaction between the nuclparallel spin I and the electron spin S of the NV.

They have the following forms:

$$H_{\mathrm{D}} = DS_z^2 + E(S_x^2 + S_y^2) \tag{4.2}$$

$$H_{\mathrm{Z}} = g\mu_B \sum_j^{x,y,z} B_j \cdot S_j \tag{4.3}$$

$$H_{\mathrm{HF}} = \vec{S} \cdot A \cdot \vec{I}. \tag{4.4}$$

Spin-Spin Interaction

The E and D in equation 4.2 the fine structure constants of the spin system, describing the spin-spin interaction and S_j the corresponding spin operators in x,y and z-direction.

D is non-zero in system with axis of threefold (or other manifold) symmetry. The symmetry or spin quantization axis points along the connection of the nitrogen atom and vacancy forming the defect. In bulk diamond D is around 2.87 GHz at room temperature.

The definiteness, orientation and magnitude of D is thus dependent on the specific spin system being studied.

E occurs when there is a distortion of the point group symmetry, for example strain or an electrical field. In bulk diamond E is typically negligibly small but especially in NDs, E can be of the order of several MHz.

Thus, similarly, the value of E is a characteristic of the nature of the distortion and the specifics of the spin system being studied.

Zeeman Interaction

B_j in equation 4.3 is the magnetic field along the x, y and z direction, g is the g-factor of the vacancy and μ_B the Bohr-Magneton, a constant.

It seems often the scaled parameter $g\mu_B$ is considered, for the NV^- system this is around 28 $\mathrm{GHz\,T^{-1}}$, but again, will be a characteristic of the system being studied.

Hyperfine Interaction

Equation 4.4 related the nuclear spin to the electron spin via the hyperfine tensor A which has the form

$$A = \begin{pmatrix} A_\perp & 0 & 0 \\ 0 & A_\perp & 0 \\ 0 & 0 & A_\parallel \end{pmatrix}. \tag{4.5}$$

$A_\parallel$ and $A_\perp$ are the axial and non-axial hyperfine parameters which encode two different interactions.

Fermi Contact Interaction. This interaction is calculated by

$$f_A = \frac{A_\parallel + 2A_\perp}{3}. \tag{4.6}$$

Anisotropic Interaction. This interaction is found by considering both spins as magnetic dipoles is calculated by

$$d_A = \frac{A_\parallel - A_\perp}{3}. \tag{4.7}$$

For the NV^- system in diamond specifically, using the values for $A_\parallel$ and $A_\perp$ we calculate that f_A is an order of magnitude stronger than d_A for both N^{14} and N^{15}.

Reduced Hamiltonian

why (specifically) do we get to neglect this? Can we generalise?

By combining H_D and H_Z and neglecting H_{HF} we find

$$H_{NV} = DS_z^2 + E(S_x^2 + S_y^2) + g\mu_B \sum_j^{x,y,z} B_j \cdot S_j \tag{4.8}$$

The spin operators S_j in matrix representation are

$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, S_y = \frac{i}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, S_z = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{4.9}$$

Then, aligning the magnetic field (with strength B_0) along the z-axis (the quantisation axis), the reduced Hamiltonian will have the form

$$H_{NV} = \begin{pmatrix} D + B_0 & 0 & E \\ 0 & 0 & 0 \\ E & 0 & D - B_0 \end{pmatrix}, \tag{4.10}$$

with Eigenvalues

$$E_x = E_y = D \pm \sqrt{B_0^2 + E^2},\ E_z = 0. \tag{4.11}$$

The corresponding non-normalised Eigenvectors are then

$$|X\rangle = \frac{1}{E}\left(B_0 + \sqrt{B_0^2 + E^2}\right)|{+1}\rangle + |{-1}\rangle \tag{4.12}$$

$$|Y\rangle = \frac{1}{E}\left(B_0 - \sqrt{B_0^2 + E^2}\right)|{+1}\rangle + |{-1}\rangle \tag{4.13}$$

$$|Z\rangle = |0\rangle, \tag{4.14}$$

with

$$|1\rangle = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}, |0\rangle = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix}, |{-1}\rangle = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}, \tag{4.15}$$

the Eigenvectors for H_{NV} with $E = 0\ldots$

In the case where $E \ll B_0$ the Eigenvectors are well described by the bases $|0\rangle$ and $|\pm 1\rangle$.

For $E \gg B_0$, when transforming the spin operators S_j into the diagonalised system with Hamiltonian H_{NV} they read

$$\hat{S}_x^{\parallel} \propto \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \hat{S}_y^{\parallel} \propto \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \hat{S}_z \propto \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \tag{4.16}$$

and

$$\hat{H}_{\mathrm{NV}} = \begin{pmatrix} D + \sqrt{B_0^2 + E^2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & D - \sqrt{B_0^2 - E^2}. \end{pmatrix} \tag{4.17}$$

Another solution for a $\pi/2$ shifted, modulating magnetic field leads to

$$\hat{S}_x^{\perp} \propto \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \hat{S}_y^{\perp} \propto \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \hat{S}_z \propto \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \tag{4.18}$$

a physical interpretation of which is that a linear modulating B-field aligned along the x-axis where strain is applied only allows transitions between the state $|X\rangle$ and $|0\rangle$, whereas fields perpendicular to the strain and the NV quantization axis only allow coupling between $|Y\rangle$ and $|0\rangle$.

For an arbitrary external magnetic field, H_{NV} can be expressed using spherical coordinates:

$$H_{\mathrm{NV}} = \begin{pmatrix} D + B_0 \cdot \cos\theta & \frac{B_0}{\sqrt{2}} \cdot e^{-i\cdot\varphi} \cdot \sin\theta & E \\ \frac{B_0}{\sqrt{2}} \cdot e^{i\cdot\varphi} \cdot \sin\theta & 0 & \frac{B_0}{\sqrt{2}} e^{-i\cdot\varphi} \cdot \sin\theta \\ E & \frac{B_0}{\sqrt{2}} \cdot e^{i\cdot\varphi} \cdot \sin\theta & D - B_0 \cdot \cos\theta \end{pmatrix} \tag{4.19}$$

Here, we transformed the magnitude of the arbitrary magnetic field into spherical coordinates as

$$B_x = B_0 \cos\varphi \sin\theta \tag{4.20}$$
$$B_y = B_0 \sin\varphi \sin\theta \tag{4.21}$$
$$B_z = B_0 \cos\theta \tag{4.22}$$

with θ the azimuthal and φ the polar angle. Then using equations 4.8 and 4.9 we compute 4.19.

It immediately follows from the characteristic equation that Eigenvalues λ satisfy

$$0 = \lambda^3 - 2\cdot\lambda^2\cdot D + \frac{D\cdot B_0^2}{2} + \lambda(D^2 - E^2 - B_0^2) - \frac{1}{2}B_0^2 \underbrace{\left(D\cdot\cos(2\theta) - 2\cdot E\cos(2\varphi)\cdot\sin(\theta)^2\right)}_{\Delta_{\varphi\theta}} \tag{4.23}$$

Chapter 5

Design

Chapter 6

Results and Analysis

Chapter 7

Conclusions

Appendix A

Python Code

'main.py'

```
import matplotlib.pyplot as plt

from sympy import Matrix
from numpy import cos, sin, sqrt, exp, linspace, pi, absolute, arccos

# DEFAULT VALUES
B_array = linspace(0, 0.01, 20)
B = 0.05
E = 0
D = 2.87 * 10**9
theta = 0  # Radians
phi = 0  # Radians


def makeMatrix(B=B, E=E, D=D, theta=theta, phi=phi) -> Matrix:
    M = Matrix(
        [
            [D + B * cos(theta), (B / sqrt(2)) *
             exp(-1j * phi) * sin(theta), E],
            [
                (B / sqrt(2)) * exp(1j * phi) * sin(theta),
                0,
                (B / sqrt(2)) * exp(-1j * phi) * sin(theta),
            ],
            [E, (B / sqrt(2)) * exp(1j * phi) *
             sin(theta), D - (B * cos(theta))],
        ]
    )
    # M = Matrix(
    #     [
    #         [D / 3 + B * cos(theta), (B / sqrt(2)) * sin(theta), 0],
    #         [
    #             (B / sqrt(2)) * sin(theta),
```

```
    #                 -2 * D / 3,
    #                 (B / sqrt(2)) * sin(theta),
    #             ],
    #             [0, (B / sqrt(2)) * sin(theta), D / 3 - (B * cos(theta))],
    #         ]
    # )
    return M


def evals(B=B, E=E, D=D, theta=theta, phi=phi) -> list:
    M = makeMatrix(B=B, E=E, D=D, theta=theta, phi=phi)
    return absolute(list(M.eigenvals().keys()))


def addToPlot(
    label, colour, opacity=0.4, B_array=B_array, E=E, D=D, theta=theta,
):
    y_array = []
    y_array.append([])
    y_array.append([])
    # y_array.append([])
    x_array = []
    # for B in B_array:
    #     es = evals(B=B, E=E, D=D, theta=theta, phi=phi)
    #     es = [num for num in es if abs(num) >= 10**7]
    #     x_array.append(B)
    #
    #     for count, e in enumerate(es):
    #         y_array[count].append(abs(e))
    #         print(count)
    #
    #     y_array[2].append(D)
    for B in B_array:
        es = sorted(evals(B=B, E=E, D=D, theta=theta, phi=phi))
        if len(es) == 2:
            es.append(es[1])

        # es = [num for num in es if abs(num) >= 10**7]
        x_array.append(B)
        y_array[0].append(abs(es[2] - es[0]))

        y_array[1].append(abs(es[1] - es[0]))
        # for count, e in enumerate(es):
        # y_array[count].append(abs(e))
    plt.plot(x_array, y_array[0], label=label, color=colour, alpha=opac
    plt.plot(x_array, y_array[1], label=label, color=colour, alpha=opac
    # plt.plot(x_array, y_array[2])
```

```
plt.xlabel("$B_0$")
plt.ylabel("Eigenvalues of $H_{NV}$")


def millerAngle(miller_1, miller_2):
    return arccos(
        [
            (
                (miller_1[0] * miller_2[0])
                + (miller_1[1] * miller_2[1])
                + (miller_1[2] * miller_2[2])
            )
            / sqrt(
                (miller_1[0] ** 2 + miller_1[1] ** 2 + miller_1[2] ** 2)
                * (miller_2[0] ** 2 + miller_2[1] ** 2 + miller_2[2] ** 2)
            )
        ]
    )[0]


applied_B_miller = (0, 0, 1)

defect_axis = (1, 1, 1)
defect_2 = (-1, 1, 1)
defect_3 = (1, -1, 1)
defect_4 = (1, 1, -1)

millerAngle(applied_B_miller, defect_axis)


addToPlot(
    label="Defect 1 $(111)$",
    colour="blue",
    opacity=0.3,
    E=0,
    theta=millerAngle(applied_B_miller, defect_axis),
)

addToPlot(
    label="Defect 2 $(\\overline{1} 11)$",
    colour="purple",
    opacity=0.3,
    E=0,
    theta=millerAngle(applied_B_miller, defect_2),
)
```

```
addToPlot(
    label="Defect 3 $(1 \\overline{1} 1)$",
    colour="green",
    opacity=0.3,
    E=0,
    theta=millerAngle(applied_B_miller, defect_3),
)

addToPlot(
    label="Defect 4 $(11\\overline{1})$",
    colour="red",
    opacity=0.3,
    E=0,
    theta=millerAngle(applied_B_miller, defect_4),
)
## Generic Results
# addToPlot(label="$E= 0, \\theta = 0$", colour="black", opacity=1, E=0
# addToPlot(
#     label="$E= 0, \\theta = \\pi/8$", colour="blue", opacity=0.5, E=0
# )
# addToPlot(label="$E= 0.005, \\theta = 0$",
#           colour="orange", opacity=0.5, E=0.005)
# addToPlot(label="$E= 0.010, \\theta = 0$",
#           colour="Purple", opacity=0.5, E=0.010)
# addToPlot(
#     label="$E= 0, \\theta = \\pi /3$", colour="green", opacity=0.5, E=
# )
#

# Diamond Results with B aligned to suface of cubic crystal
# addToPlot(label="$E= 0, \\theta = 0.927$",
#           colour="blue", opacity=0.8, E=0, theta=0.927)
# addToPlot(label="$E= 0, \\theta = 2.214$",
#           colour="blue", opacity=0.8, E=0, theta=2.214)
#
# Diamond results with B aligned to [210] (to generate 4 different angl

# addToPlot(label="$E= 0, \\theta = 0.68$",
#           colour="blue", opacity=0.5, E=0, theta=0.68)
#
# addToPlot(label="$E= 0, \\theta = 1.83$",
#           colour="blue", opacity=0.5, theta=1.83)
#
# addToPlot(label="$E= 0, \\theta = 1.31$",
#           colour="blue", opacity=0.5, E=0, theta=1.31)
#
# addToPlot(label="Base", colour="black", opacity=1, E=0, theta=0.927)
# addToPlot(label="Base", colour="black", opacity=1, E=0, theta=5.355)
```

```
# addToPlot(label="Base", colour="black", opacity=1, E=0, theta=2.214)
# addToPlot(label="Base", colour="black", opacity=1, E=0, theta=4.069)
# addToPlot(label="Base", colour="black", opacity=1, E=0, theta=pi / 4)
# addToPlot(label="Base Lower D", colour="black",
# opacity=1, D=2.6 * 10**9, theta=0)
# addToPlot(label="Base, $E=50$", colour="green", E=5 * 10**6, theta=0)
# addToPlot(label="Base, $E=50$", colour="green", E=5 * 10**6, theta=pi * 0.
# addToPlot(label="Base, $E=500$", colour="blue", E=9 * 10**6, theta=0)

#
handles, labels = plt.gca().get_legend_handles_labels()
by_label = dict(zip(labels, handles))
plt.legend(by_label.values(), by_label.keys())
plt.title("$B_0$ aligned with " + "".join(map(str, applied_B_miller)))
plt.xlim(left=0)
plt.show()
```

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