



NQR USING N-V COLOR CENTER

Naman Pagaria¹, Mimansa Pandey¹, Sameera Khan²

B.Tech, Computer Science Engineering, Amity University Chhattisgarh, Raipur, India¹

Assistant Professor, Amity School of Engineering and Technology, Amity University Chhattisgarh, Raipur, India²

Abstract: Nitrogen vacancy (NV) centre is a small imperfection in the structure of diamond. These NV centres due to their unique properties find applications in various fields like magnetometry, Nano-MRI etc. This is why it is considered to be one of the most promising new technologies for the future of nanoscale magnetic measurements and imaging. N-V colour centres in a diamond lattice are of utmost significance due to their photoluminescence properties. It can achieve significantly high degree of spin polarization with optical illumination. In addition to the defect's quantum spin states interacting with magnetic fields, the spin state of N-V centres is especially long lived and provides a long coherence time to allow magnetometry with the ability to remain intact up to a few milliseconds at room temperature. This paper throws light on various concepts related to Nuclear Quadrupole resonance (NQR) with respect to NV colour centres in the diamond lattice. In future, the use of these individual, atomic-sized quantum systems can thereby be used inspire new concepts in the fields of cell biology and solid-state physics too.

Keywords: Nitrogen vacancy, magnetometry, photoluminescence, quantum spin, Nuclear Quadrupole resonance.

I. INTRODUCTION

Looking at a crystal defect as a tool for spatial nanoscale measurement tool is not an instinctive choice however, Magnetic resonance spectroscopy (EPR, NMR) is one of the most important tools used today for complex structural determination at a molecular level, but it is typically only restricted and limited to observables at a macroscopic scale. Henceforth it extremely challenging to characterize and analyses electronic properties for two dimensional materials such as graphene.

The Understanding of these nanometre-scalic two-dimensional materials is an absolute necessity for the exploration of condensed matter phenomena and for the development of necessary technological applications, this can be assuredly obtained via advance nanometre-scalic nuclear quadrupole resonance (NQR) spectroscopic techniques using the N-V colour centre point defect in high purity diamonds.

Meticulous manipulation of these colour centres and the usage of these sensors, consisting and comprising of two quantum bits, one for electronic spin and the other for ancillary nuclear spin respectively at stable room temperatures can enable magnetic resonance detection and spectroscopy of nuclear species. Quantum logic is consistently used to improve the readout fidelity and spin coherence time and it is extended by the use of nitrogen-vacancy centres. The aggregate gain in this sensitivity is ample to detect complex nanoscale structures of individual proteins and could be supplementary used to reveal additional details on its chemical composition.

On demonstration of Magnetic resonance imaging operating on the surface of a high purity diamond availing isolated electronic-spin qubits as magnetic resonance reporters under preferable and ambient conditions while delimitating these spin qubits with nanometre-scale uncertainty.

The quantum state of these spin qubits often optically measured using an N-V colour centre located a few nanometres below the diamonds surface. Furthermore, this system is used for individual imaging of proton spins with angstrom resolution and can be also be used for complex nanoscale structural imaging of bulk molecules. NMR schemes constructed on nitrogen vacancies in high purity diamond surfaces can be used to initiate complex nanoscale images of spins of individual protons and manipulation of complex quantum level surfaces.

II. SETUP

The NV Centres are created imminently to the diamonds surface (depth < 10nm), and the sample of the 2d material is kept precisely on the diamond surface. The NV Centre is carefully examined using amalgamation of microwaves and laser light so as to bloat the sensitivity to the NQR frequencies of interest. The proximity of the sensor to the examined



sample is largely boosted, enabling the detection of NQR signals even from samples that are only a few atomic layers capacious.

Under favoured conditions, coherent control of individual N-V centre is used for label-free detection of nuclear polarization of nanoscale entities. Negatively charged N-V centre has an extensively long coherent time, spreading up to a few nanoseconds, even at room temperature and it provides efficient, all-optical spin polarization due to its electronic level structure. Fourier components of various magnetic discipline created with the aid of statistically polarized subset of proximal nuclear spins contained within a protein is measured. The spin magnetization of the spin undergoes precession on the Lamour frequency/ Precessional frequency with segment and amplitude that vary in accordance to each repetition. Zero mean magnetization with a nonzero variance is acquired by averaging over many iterations which ends up in a measurable magnetic resonance signal.

The spin state of the NV centre is manipulated with a series of periodic microwave pulses separated through unfastened-evolution durations of length τ . As a end result of this periodic modulation, a slim band-bypass frequency filter is created. This permits for phase accumulation when the modulation frequency, defined as $1/\tau$, is close to two times the nuclear Precessional frequency. A frequency spectrum capable of encoding information about the nuclear spins inside the protein is yielded by using varying spacing between the π pulses.

Optimal sensitivity of this technique is acquired when the pulse-sequence period is about identical to the coherence time T_2 of the NV electronic spin. Readout fidelity encapsulates the impact of photon shot noise and approaches unity for an ideal, projection noise-limited dimension.

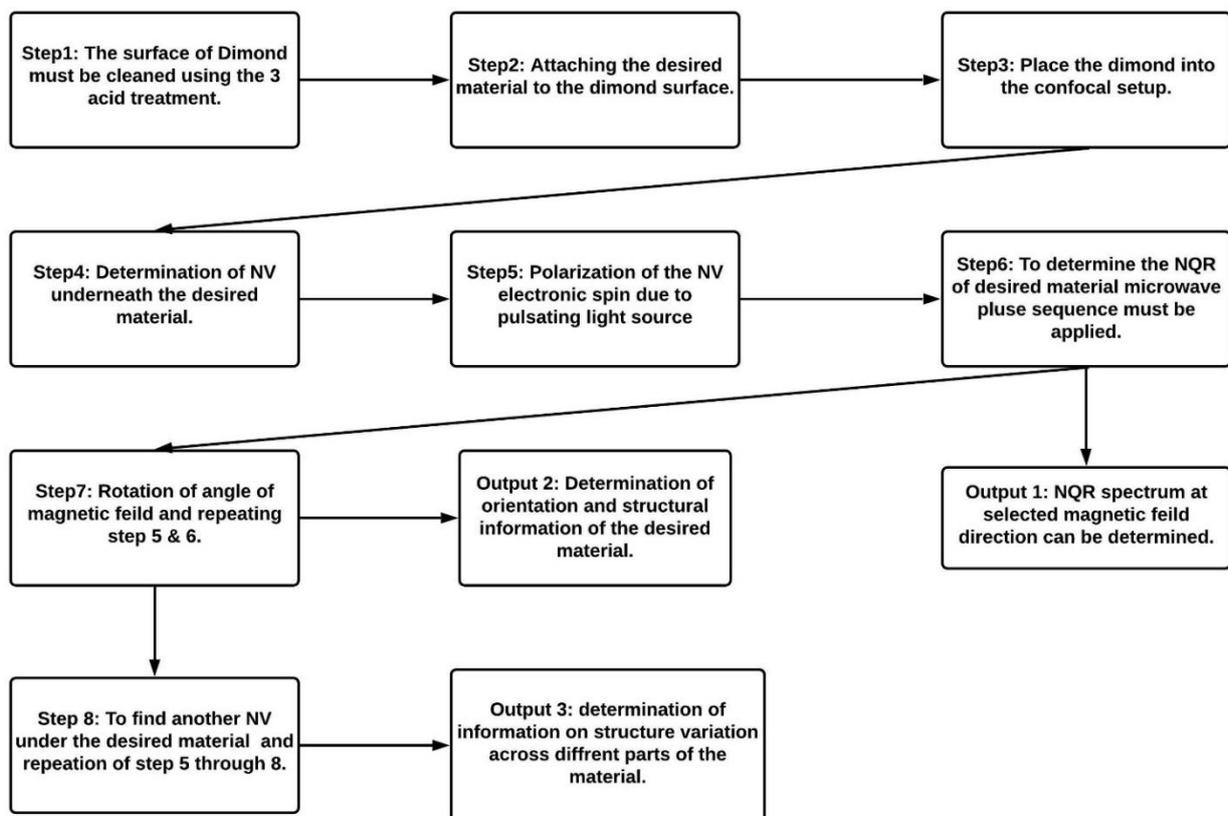


Figure 1(stepwise description of the process)



III.WORKING

Under preferable conditions, coherent control of individual N-V centre is used for label-free detection of nuclear polarisation of nanoscale entities.

Negatively charged N-V Centre has an incredibly long coherent time, even at room temperature and it provides efficient, all-optical spin polarisation due to its electronic level structure.

Fourier components of varying magnetic field created by statistically polarized subset of proximal nuclear spins contained within a protein is measured.

The spin magnetization of the spin is subject to a precession at the Lamour frequency / processional frequency with phase and amplitude that vary depending on the repetition.

Zero mean magnetisation with a nonzero variance is obtained by averaging over many iterations which results in a measurable magnetic resonance signal.

The spin state of the NV Centre is manipulated with a series of periodic microwave pulses separated by free-evolution intervals of length τ .

As a result of this periodic modulation, a narrow band-pass frequency filter is created. This allows phase accumulation when the modulation frequency, defined as $1/\tau$, is close to twice the nuclear Processional frequency.

A frequency spectrum capable of encoding information about the nuclear spins within the protein is yielded by varying the spacing between the π pulses.

Optimal sensitivity of this technique is obtained when the pulse-sequence duration is approximately equal to the coherence time T_2 of the NV electronic spin.

The readout fidelity encapsulates the effect of photon firing noise and is almost one for an ideal measurement that is limited by projection noise.

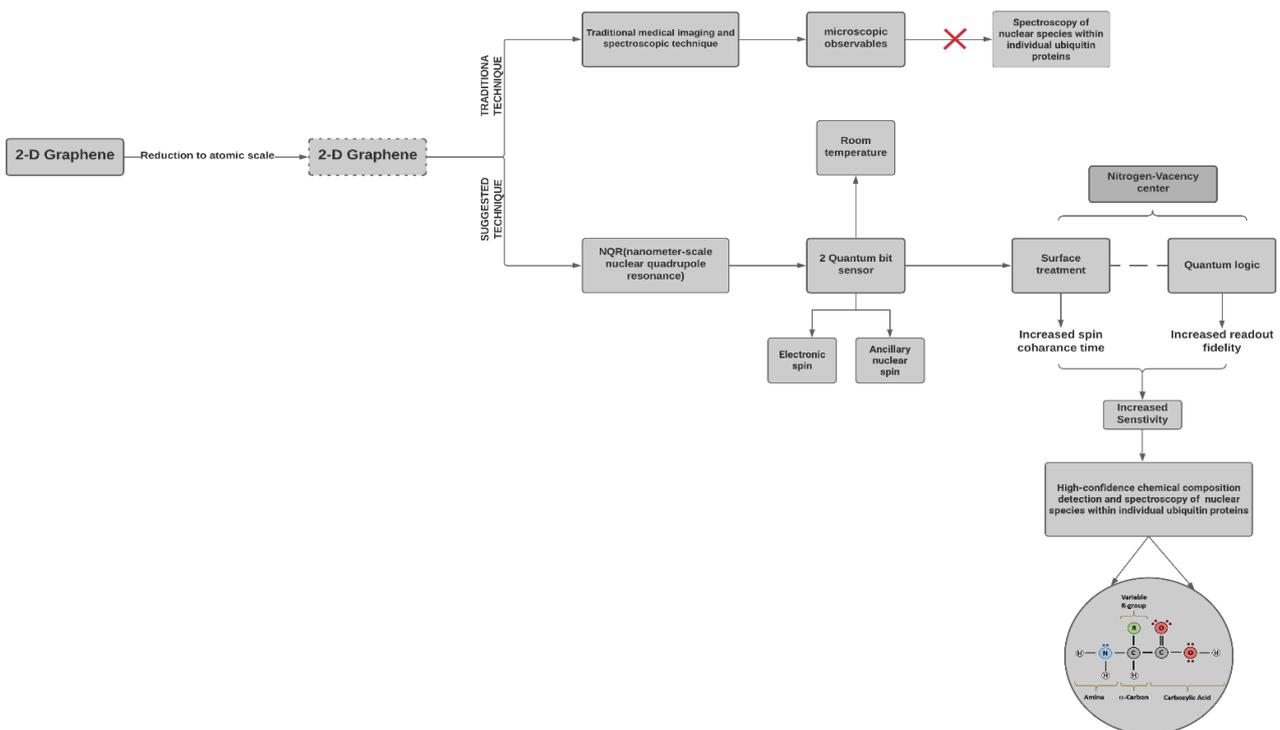


Figure 2 (Block diagram of the working)

IV. IDENTIFICATION OF PROCESSIONAL FREQUENCY AND EFFECTIVE MAGNETIC FIELD

The working of an NMR can be observed by identifying the following parameters:

I (Spin quantum number) = $\frac{1}{2}$

S (Spin angular momentum) = $\frac{h}{2\pi}I$

m (magnetic moment) = $2I + 1$

μ (magnetic momentum) = $\gamma * S$

E (Magnetic energy) = $\mu * B_0$

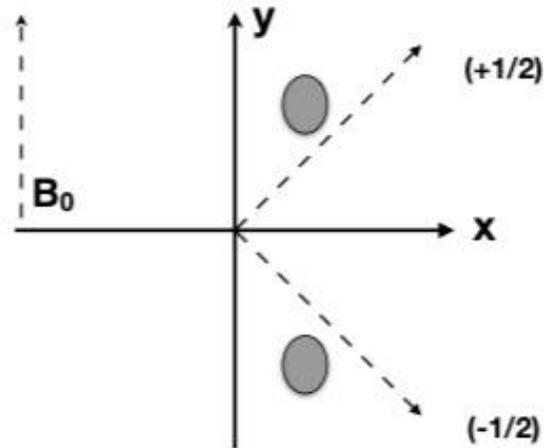


Figure 3(Identification of magnetic energy)

When, $I = \frac{1}{2}$,

$m = 2(I) + 1 = 2; +1/2, -1/2$

$S_{+1/2} = \frac{h}{2\pi} (+1/2) = +\frac{h}{4\pi}$

$S_{-1/2} = \frac{h}{2\pi} (-1/2) = -\frac{h}{4\pi}$

$\mu_{+1/2} = \gamma * S_{+1/2} = +\gamma h/4\pi$

$\mu_{-1/2} = \gamma * S_{-1/2} = -\gamma h/4\pi$

$E_{+1/2} = \mu_{+1/2} * B_0 = +\gamma h B_0/4\pi$

$E_{-1/2} = \mu_{-1/2} * B_0 = -\gamma h B_0/4\pi$

$\Delta E = E_{-1/2} - E_{+1/2}$

$\Delta E = -\gamma h B_0/2\pi$

$\Delta E = h\nu$

$-\gamma h B_0/2\pi = h\nu$

$\gamma B_0/2\pi = \nu$ (only magnitude is considered)

$\nu = \gamma h B_0/2\pi$ (Processional frequency)

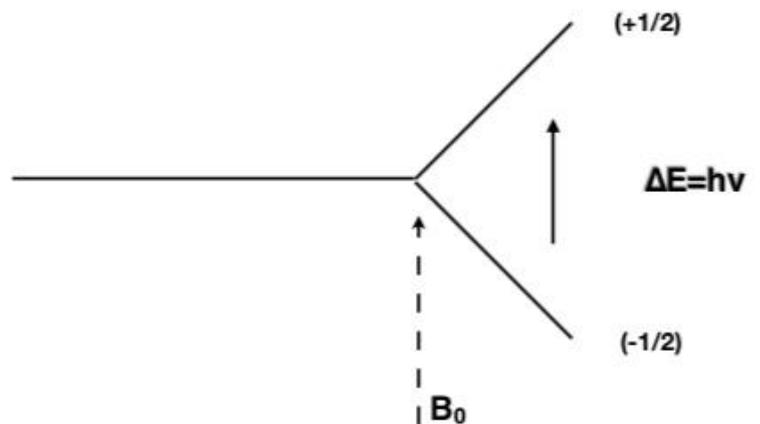


Figure 4(Identification of processional frequency)



V. SPIN DEPENDENT FLUORESCENT PROPERTY OF N-V CENTRE

Generation of luminescence through excitation of a molecule by ultraviolet or visible light photons is a phenomenon termed photoluminescence, which is formally divided into two categories, fluorescence and phosphorescence, depending upon the electronic configuration of the excited state and the emission pathway.

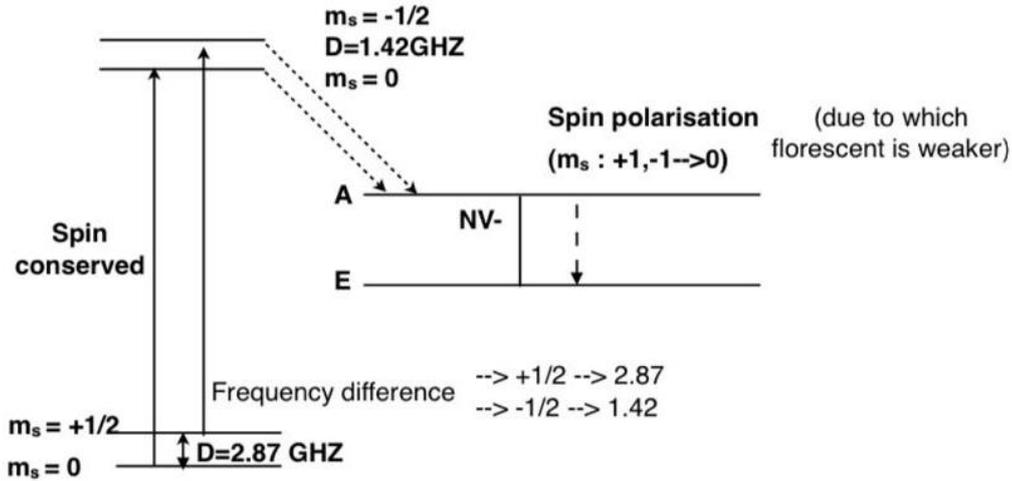


Figure 5(Identification of magnetic field with the use of Electro paramagnetic resonance)

Therefore, the application of magnetic field results in Zeeman effect and splits the spectrum line into several components, this makes the N-V Centre a stable source of Single Photon emission at room temperature.

As the magnetic field is applied it gives a rise to spin dependent fluorescent property of the NV centre, the change in the magnetic field can be calculated with the change in intensity.

To measure the magnetic field with high sensitivity and Nano scale spatial resolution a microwave field is optically used over the Electro paramagnetic resonance and makes it possible to utilise the N-V centres and these N-V centres helps to find accurate measurements for finding magnetic field.

Properties of N-V Centre for its spin dependent florescent structure -

- * N-V centres are photo-luminescent in nature and they can easily be individually detected with conventional microscopy.
- * N-V centres are easily operable at room temperature; temperature control is not required.

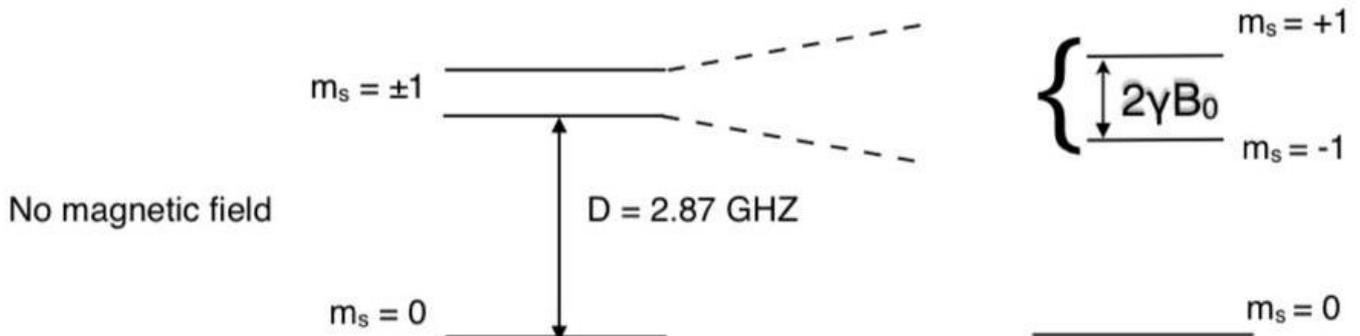


Figure 6 (Spin depended florescent proper)



VI. OPTIMAL SENSITIVITY & READOUT FIDELITY

- Optimal Sensitivity - defined by the least number of nuclear spins(N) detectable after 1s of integration.
- Where,

$$N \approx \frac{16\pi^4 d^6}{(\mu_0 \hbar \gamma_e \gamma_n)^2 F} \frac{\sqrt{T_2 + T_R}}{T_2^2}$$

- Here,
- $\gamma_e = 1.76 \times 10^{11} \text{ s}^{-1} \text{ T}^{-1}$
-
- for proton spins, $\gamma_n = 2.68 \times 10^8 \text{ s}^{-1} \text{ T}^{-1}$ (electron and nuclear gyromagnetic ratios)
- d - depth of the N-V centre,
- μ_0 - vacuum permeability,
- \hbar - Planck's constant ($\hbar/2\pi$)
- T_R is the readout time.
- F - Readout fidelity (determined by mean number of photons α_0, α_1 detected per shot from the $m_s = 0$ and 1 spin sublevels of the NV centre)

$$\mathcal{F} = \left[1 + 2(\alpha_0 + \alpha_1) / (\alpha_0 + \alpha_1)^2 \right]^{-\frac{1}{2}}$$

VII. CONCLUSION

The restricted measurement skills of current day Magnetic resonance spectroscopic tools inclusive of EPR, NMR makes it strenuous to perform particular analysis of large complicated molecules. Structure-resolving magnetic resonance spectroscopy can be tested with the use of Nitrogen-vacancy centres in high purity diamonds due to its optically addressable single-spin magnetometer property which could initially be used for rudimentary NMR spectroscopy of nanoscale samples.

In preliminary stages, molecular qubits can be used for hosting stable unpaired electrons and can be similarly used as spin labels to image more complex molecules such as proteins. These molecular qubits may be assembled into dipolar-interacting spin networks of our required geometry and length. Quantum control over these geometric networks with the use of N-V centre can prove to be a promising system for analysing nanoscale quantum dynamics.

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