Data Assimilation For Quantum Nitrogen Vacancy (NV) Spectroscopy

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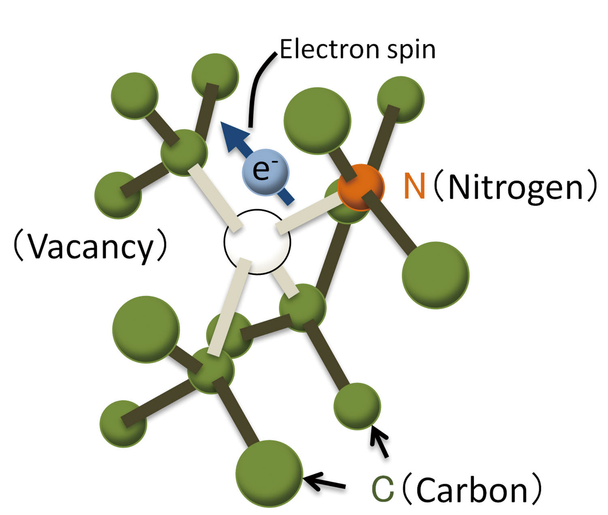
Introduction

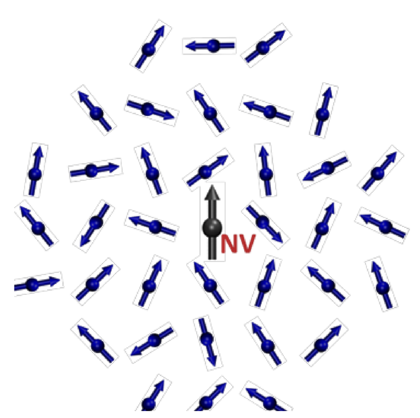


A Nitrogen Vacancy Center

- **NV** • Point Defect in Diamond
- **Goal** • To develop a primary sensor
- **Strategy** • Construct a statistical model

Pure Diamond

Yellow Color due to Nitrogen Impurities



Spin Dynamics

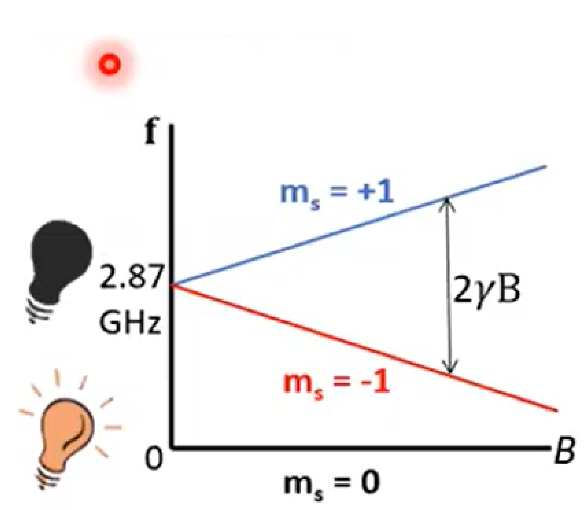
Background

Ground State

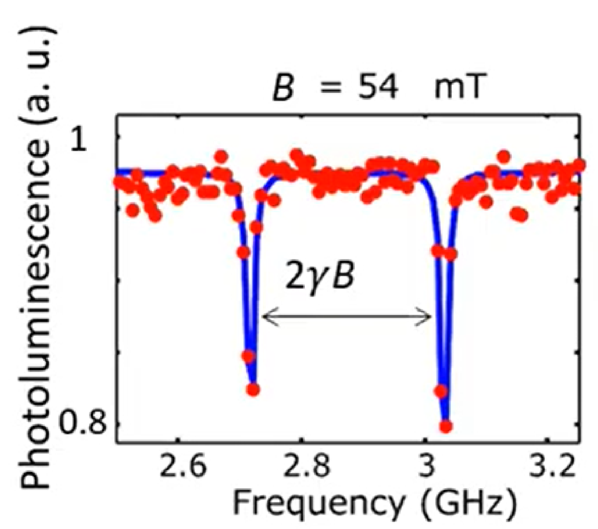
Excited State

Singlet State

Electronic Levels



Zeeman Splitting



Resonance Spectra

Hamiltonian

- Hamiltonian:

$$\hat{H} = \hbar D\left[\hat{S}_Z^2 - \frac{2}{3}\right] + \hbar E\left(\hat{S}_X^2 - \hat{S}_Y^2\right)$$

- $\hbar$: Planck's constant
- $D,\ E$: Zero-Field Parameters
- Spin Operators:

$$\hat{S}_X = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \hat{S}_Y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \hat{S}_Z = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Statistical Model

Goal: To compute the best estimators for temperature and pressure.

1. Measurements for D & E
2. Compute Hamiltonian
3. Obtain the Power Spectrum
4. MLE for Temperature & Pressure

Temperature Pressure Influence

$$D = aT + b + \alpha(P - P_0)$$

$$E = cT + d + w$$

Power Spectrum

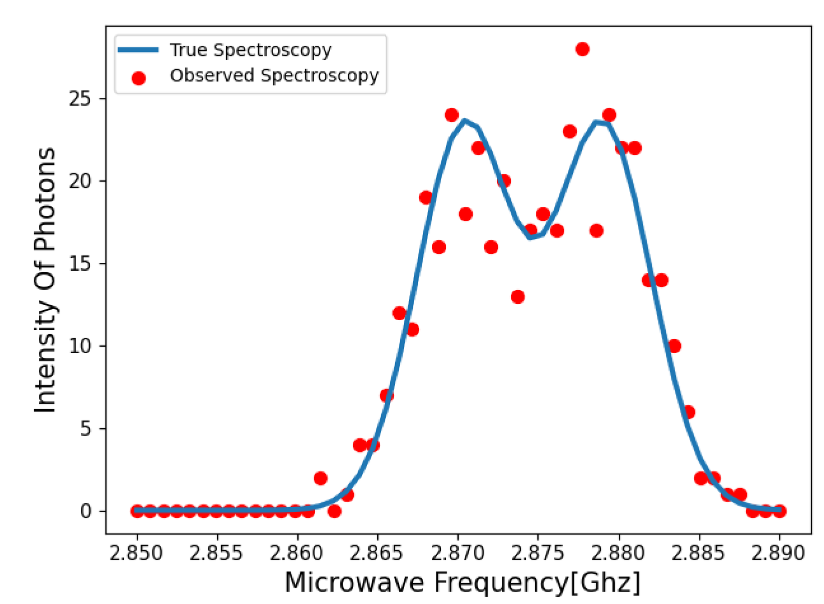
The Schrödinger's Equation

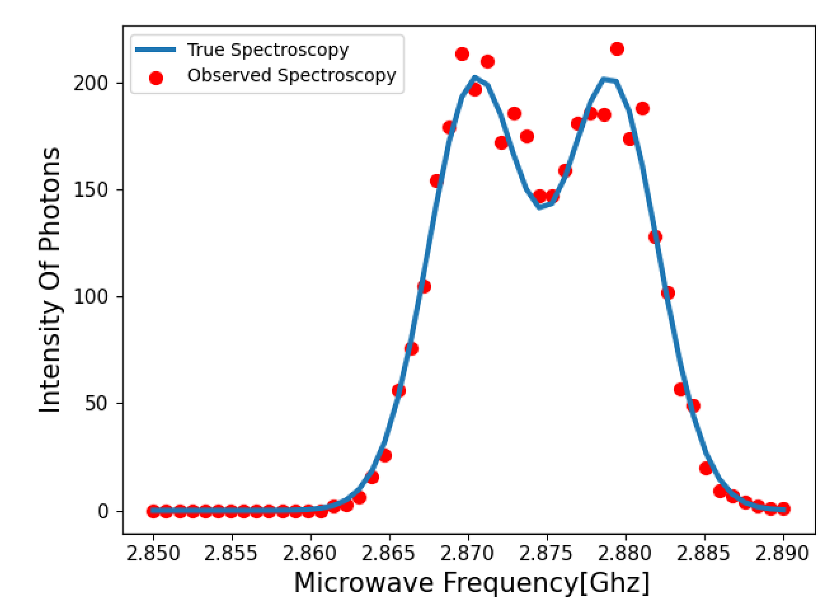
$$\iota\hbar\frac{\partial\Psi(x,t)}{\partial t} = \hat{H}(\Psi)(x,t)$$

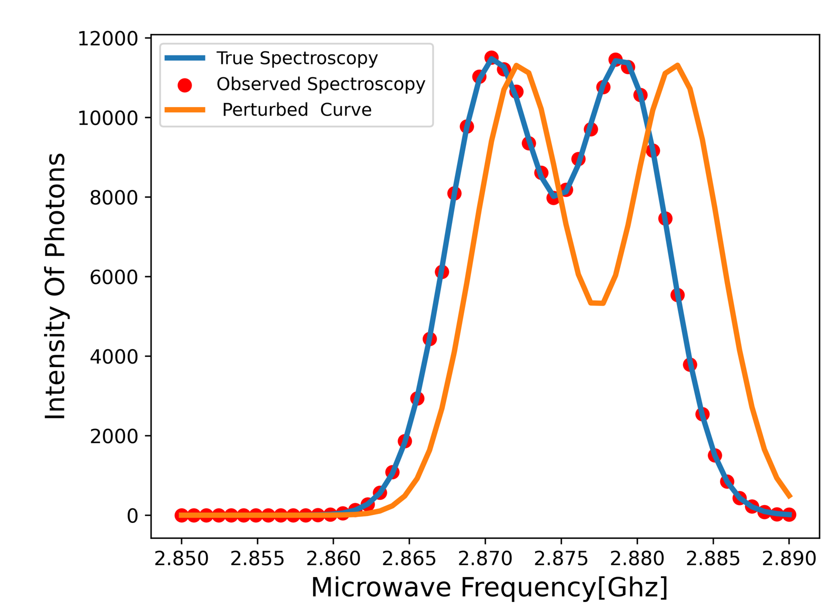
Power Spectrum

$$P(w) = |\hat{\Psi}(w)|^2 = \hat{\Psi}(w)^*\hat{\Psi}(w)$$

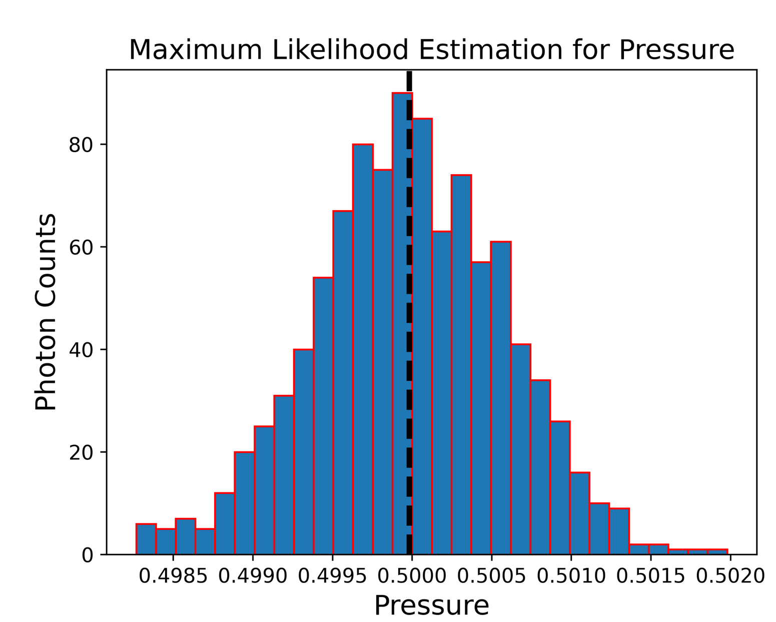
Zero Field Spectra and Independent Poisson Random Variables

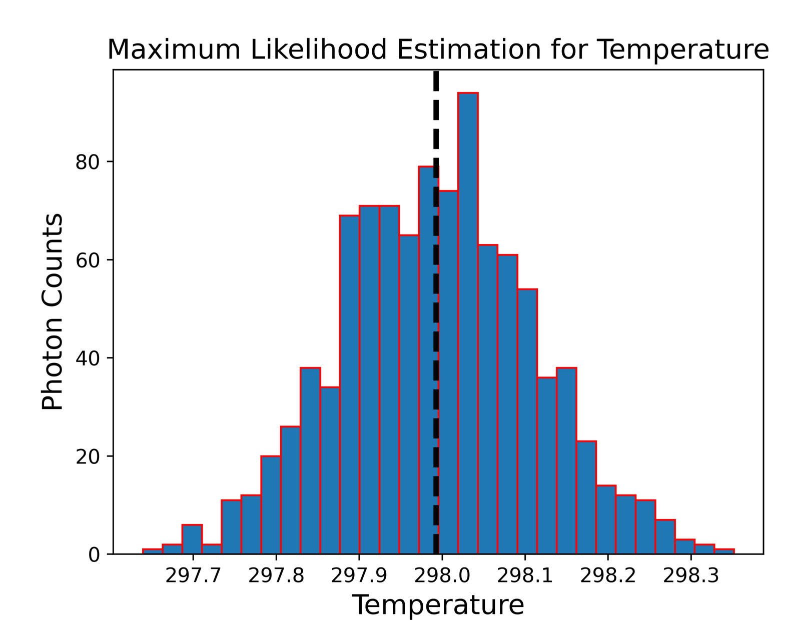


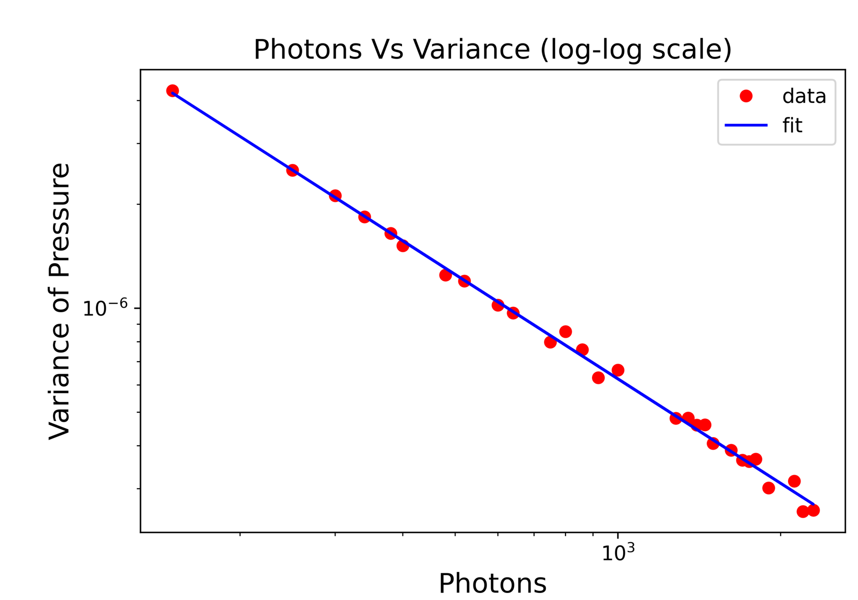


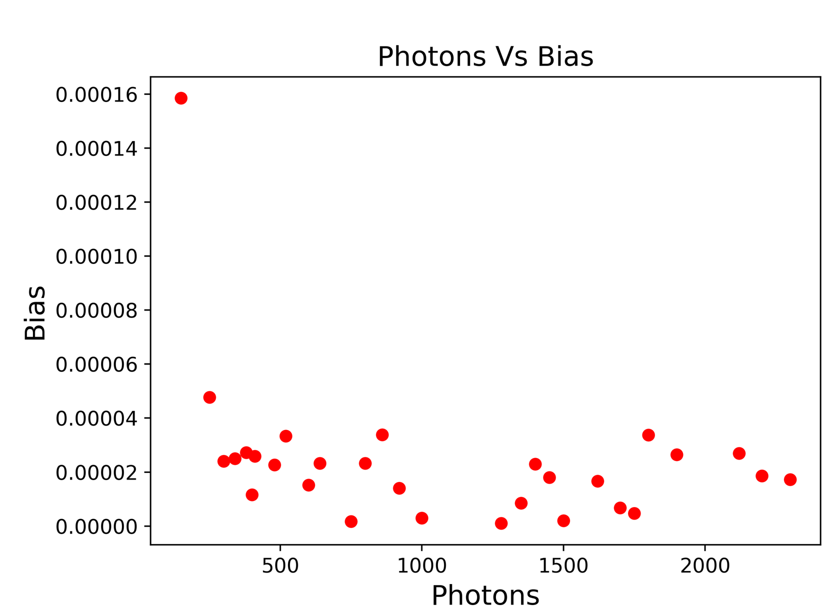


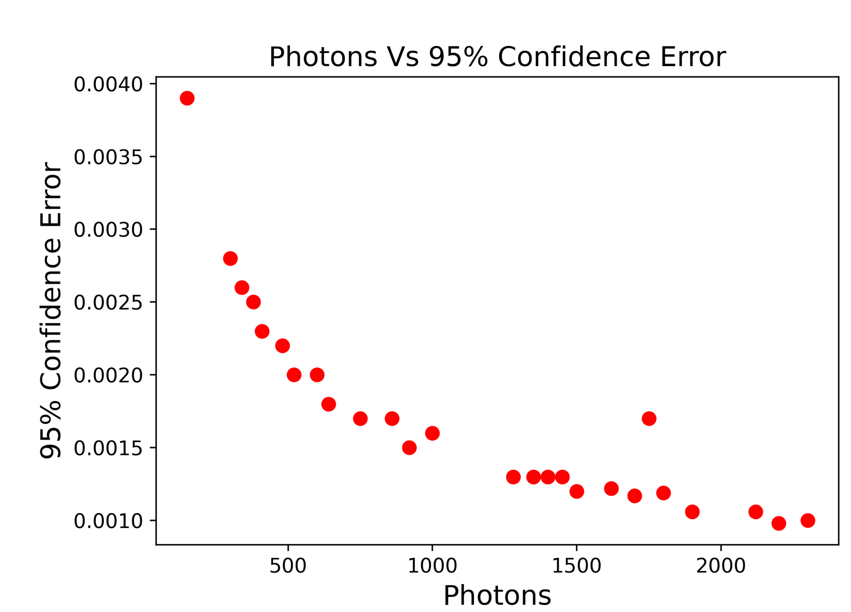
Experiments and Sensitivity Analysis

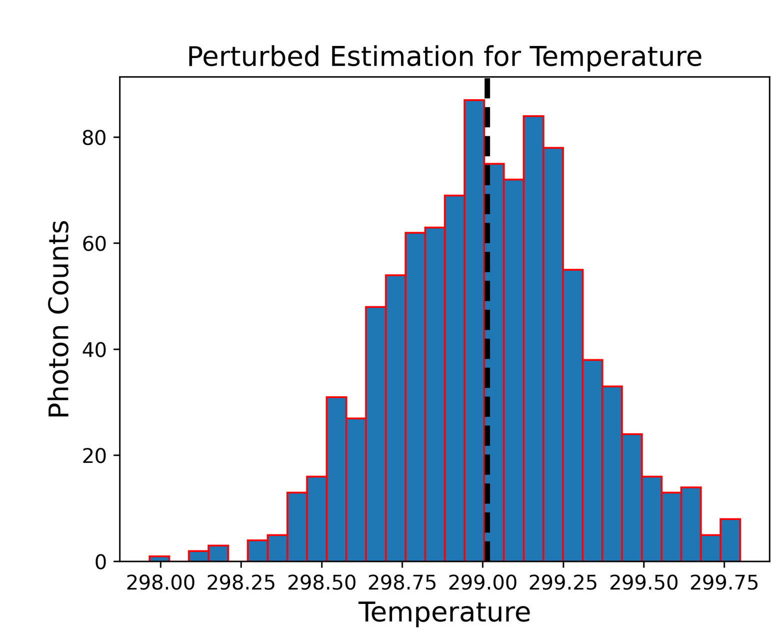












Maximum Likelihood Estimation

- Q_k : Poisson Variable
- m : Photons
- r : Rate of Photons
- S : Spectroscopy Curve
- $\gamma = \Delta t r S(\omega_k)$: Poisson Rate
- Likelihood for Poisson Variable :

$$S(Q_k = m \mid \gamma) = \frac{\gamma^m e^{-\gamma}}{m!} = \frac{(\Delta t r S(\omega_k))^m e^{-\Delta t r S(\omega_k)}}{m!}$$

$$S(Q_k = m \mid T, P) = \frac{(\Delta t r \mathcal{S}_k(T,P))^m e^{-\Delta t r \mathcal{S}_k(T,P)}}{m!}$$

- Log Likelihood function of the Spectroscopy Curve :

$$\log(\mathrm{S} \mid T, P) = \sum_{k=1}^{N} m_k \log(\Delta t r \mathcal{S}_k(T,P)) - \Delta t r \mathcal{S}_k(T,P) - \log(m_k!)$$

-LogLikelihood → Gradient → Hessian → MultiVariate Newton's Method

Conclusions and Future Work

Conclusions:

- The optimal measurements for temperature and pressure have been identified.
- Estimated mean temperature and pressure was comparable to true temperature and true pressure.
- Increasing rate of photons reduces the variance of estimate error.
- Results of sensitivity analysis show that our method is robust to the small violations of assumptions.

Future Work:

- Incorporating data assimilation methodology to be able to update our estimate in real time.
- Use training reference data to build model estimators ; a,b,c,d and alpha.

Acknowledgements

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References

[1] Phila Rembold, Nimba Oshnik, Matthias M. Müller, Simone Montangero, Tommaso Calarco, Elke Neu, et al. *Introduction to quantum optimal control for quantum sensing with nitrogen-vacancy centers in diamond* .

[2] Yan-Kai Tzeng, Pei-Chang Tsai, Hsiou-Yuan Liu, Oliver Y. Chen,Hsiang Hsu, Fu-Goul Yee, Ming-Shien Chang,*, and Huan-Cheng Chang,**Time-Resolved Luminescence Nanothermometry with Nitrogen- Vacancy Centers in Nanodiamonds*.