

# Simphony

our python package to simulate  
point defect dynamics



ReAQCT, Budapest, June 19 2024

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Budapest, Hungary

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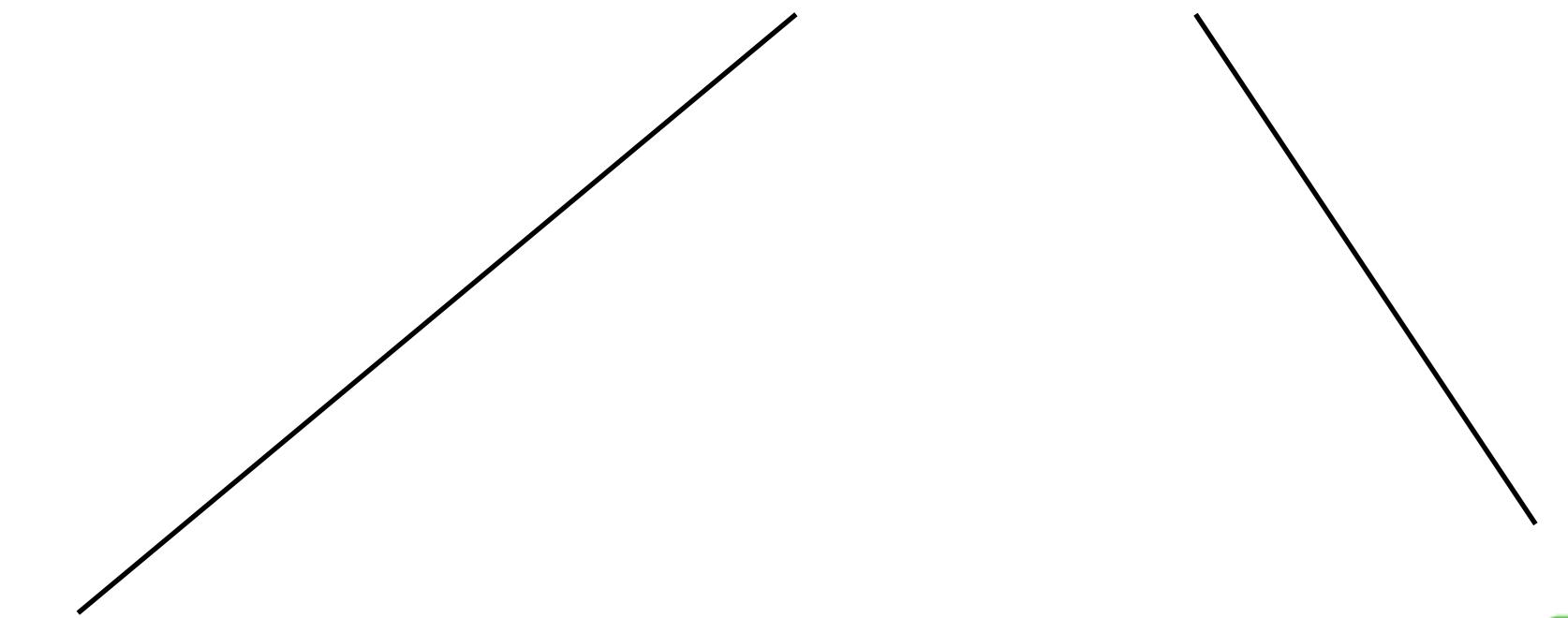


Qutility

# Funding acknowledgment



AI4QT



NATIONAL RESEARCH,  
DEVELOPMENT  
AND INNOVATION OFFICE  
HUNGARY



PROJECT  
FINANCED FROM  
THE NRDI FUND



eureka  
innovation beyond borders

# AI4QT partners (Hungary, Germany)



# Simphony



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qutility.io

Our python package to simulate point defect quantum dynamics  
for quantum technology applications

## Quantum Computing

*Universal high-fidelity quantum gates  
for spin-qubits in diamond*

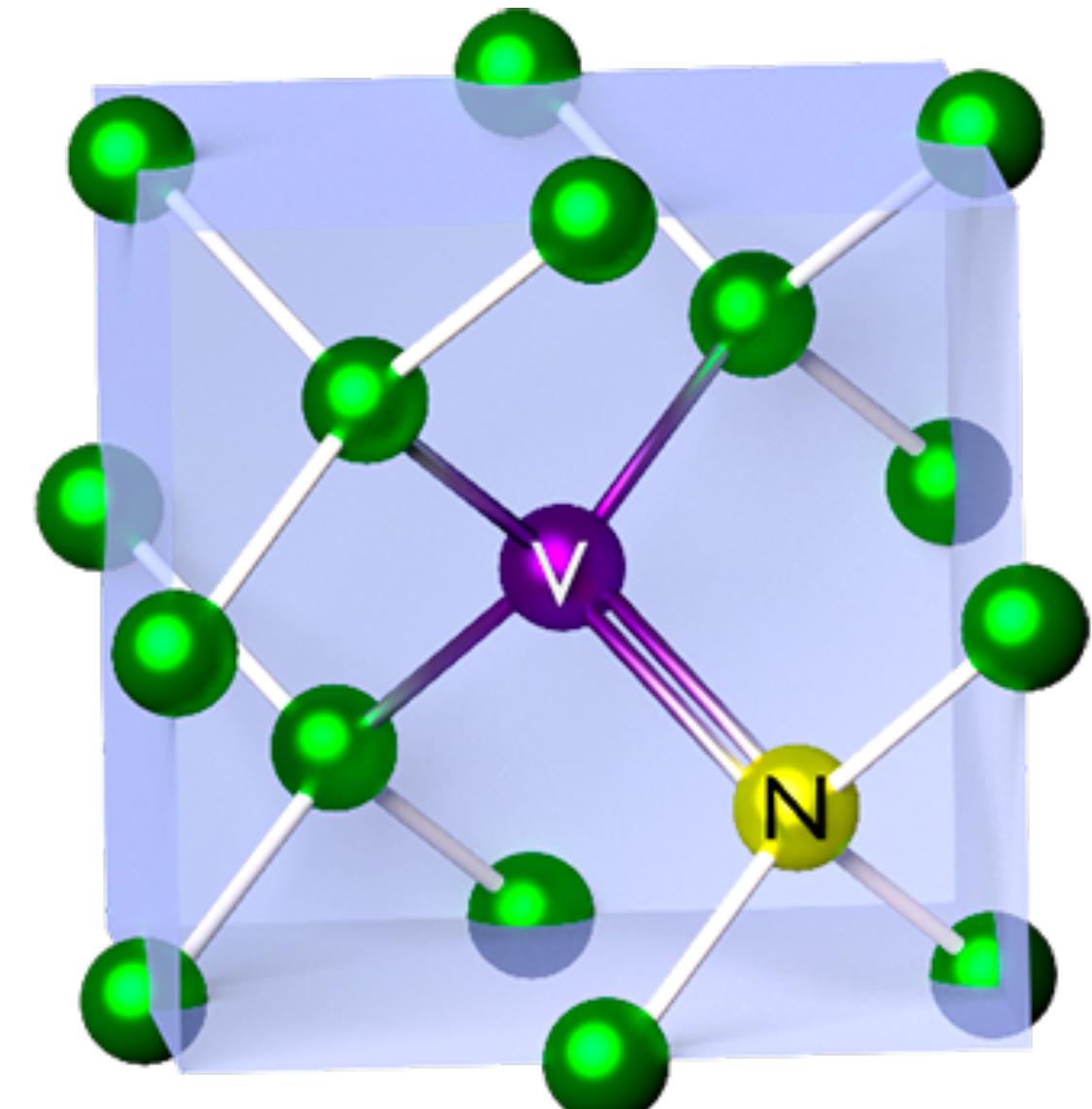
<https://arxiv.org/abs/2403.10633>

Taminiau group, Delft

*High-Fidelity Electron Spin Gates  
in a Scalable Diamond Quantum Register*

<https://arxiv.org/abs/2406.04199>

Jelezko group, Ulm



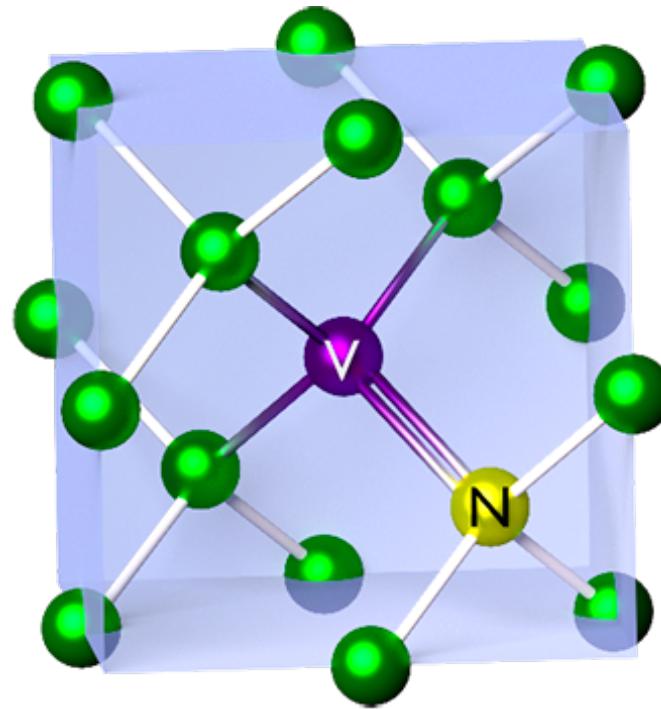
## Quantum Sensing

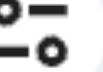
*Nanoscale magnetism and magnetic  
phase transitions in atomically thin CrSBr*

<https://arxiv.org/abs/2312.09279>

Maletinsky group, Basel

# Simphony



 [qutility.io](https://github.com/qutility)

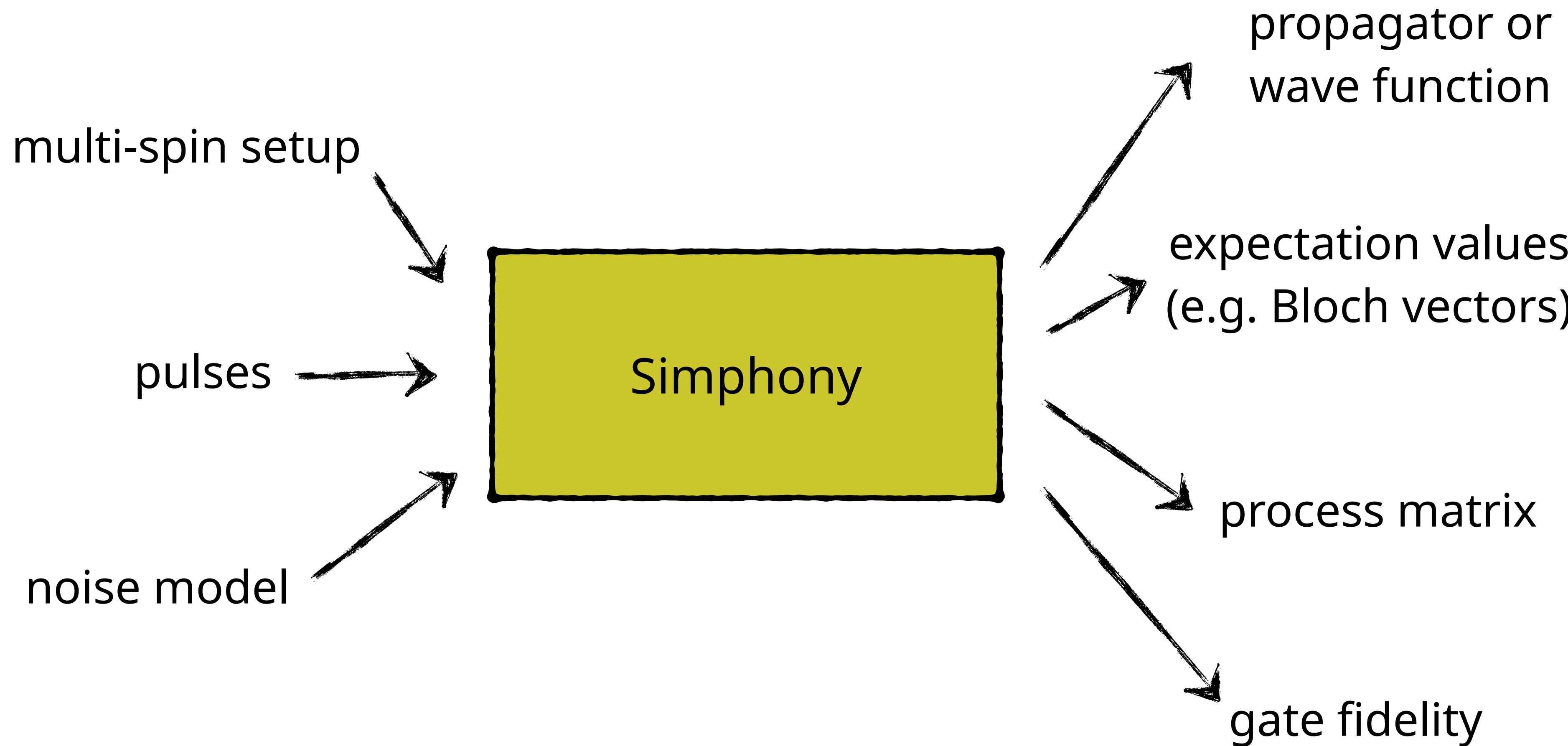
- Simphony is our python package to simulate point defect quantum dynamics for quantum technology applications
- Simphony is our “Minimal Viable Product” => **We are looking for collaborators!**



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# Input-output structure of Simphony

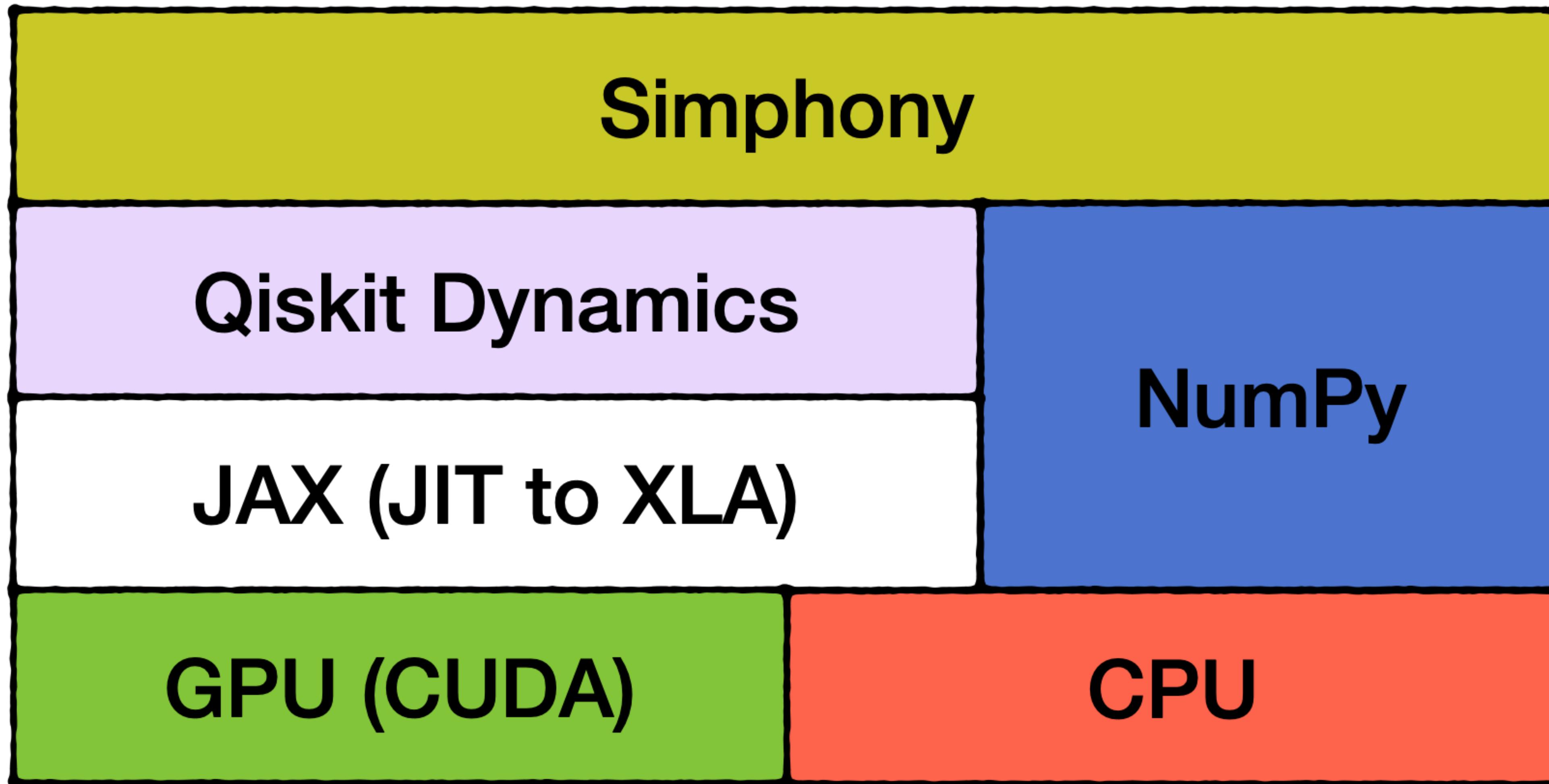




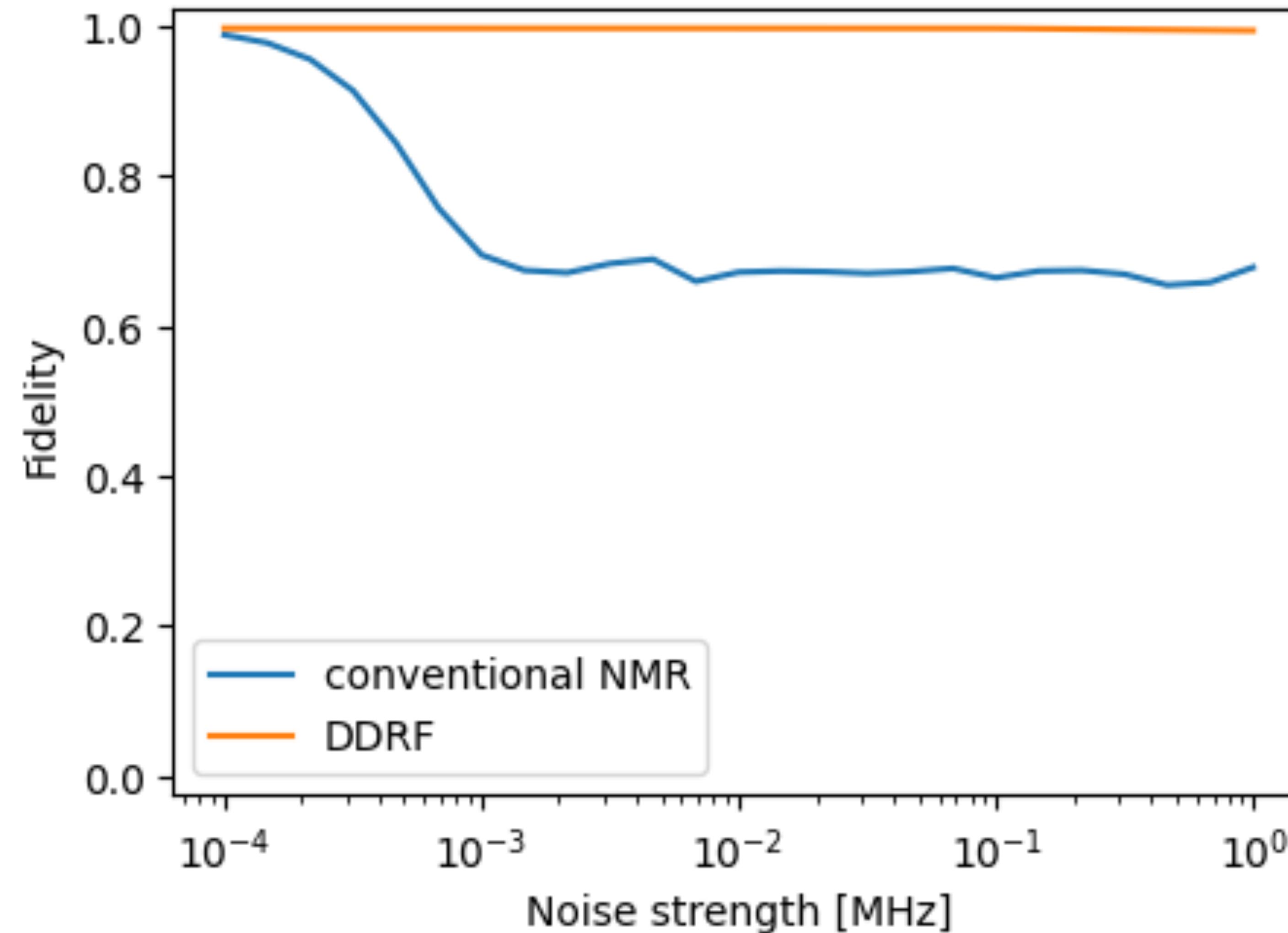
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# Dependency diagram of Simphony

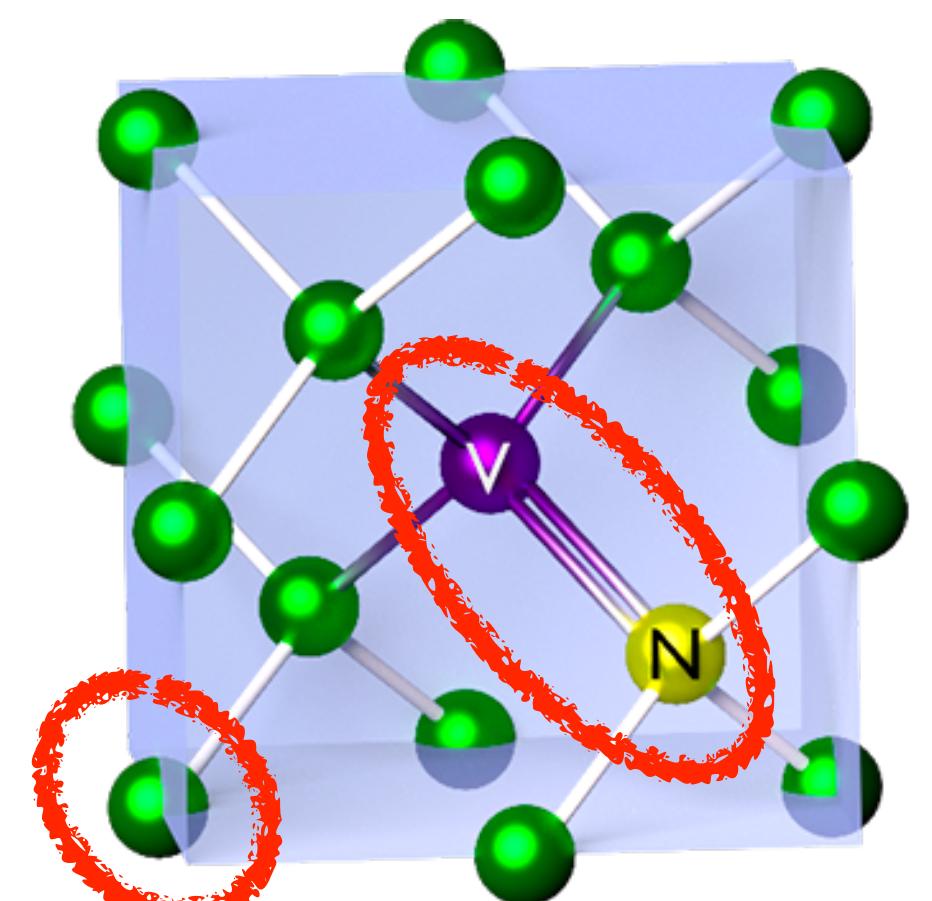
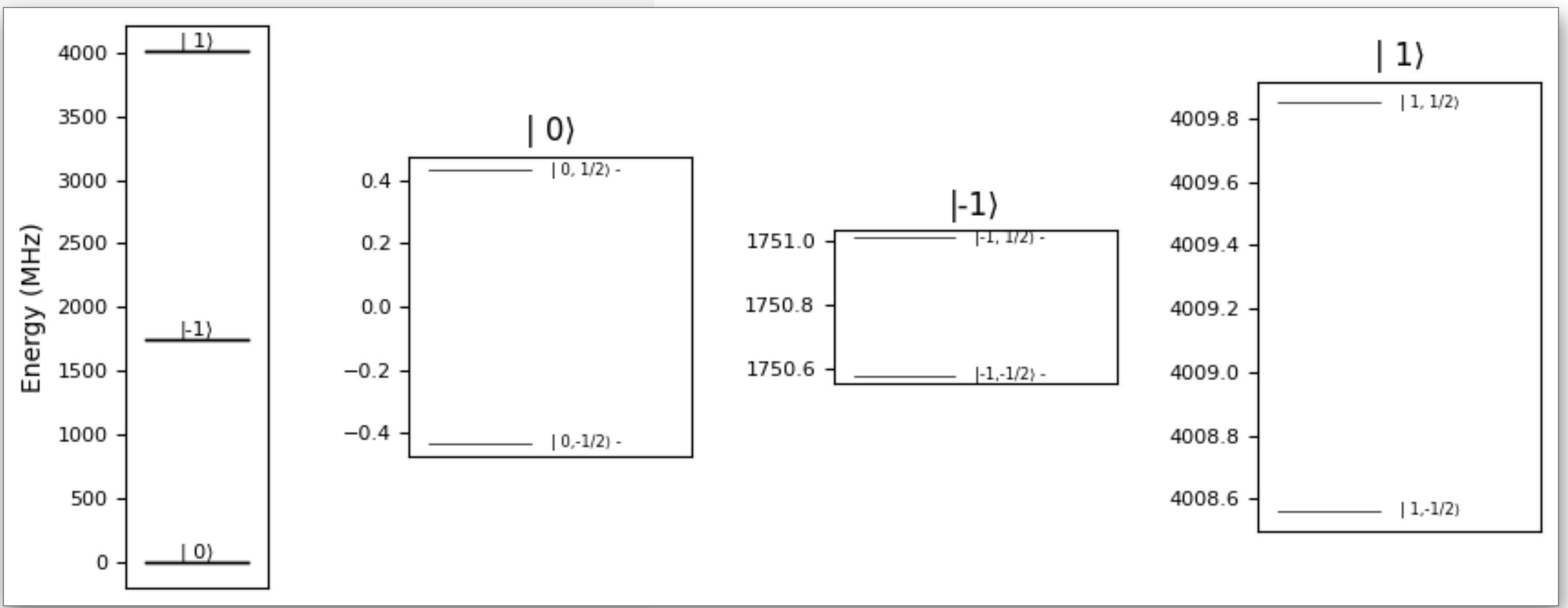


# Example: noise-resistant controlled rotation

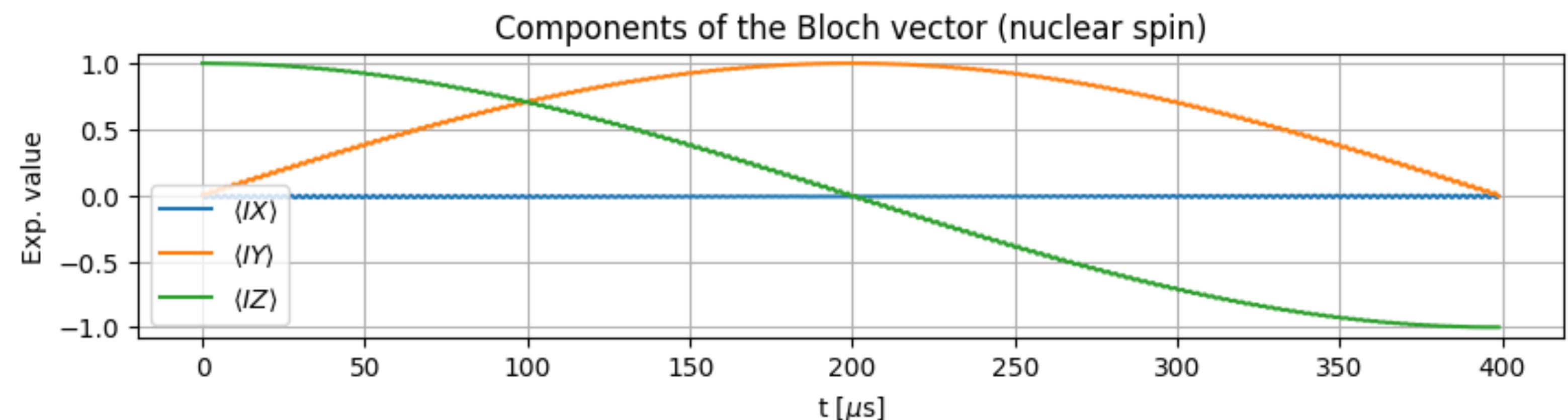
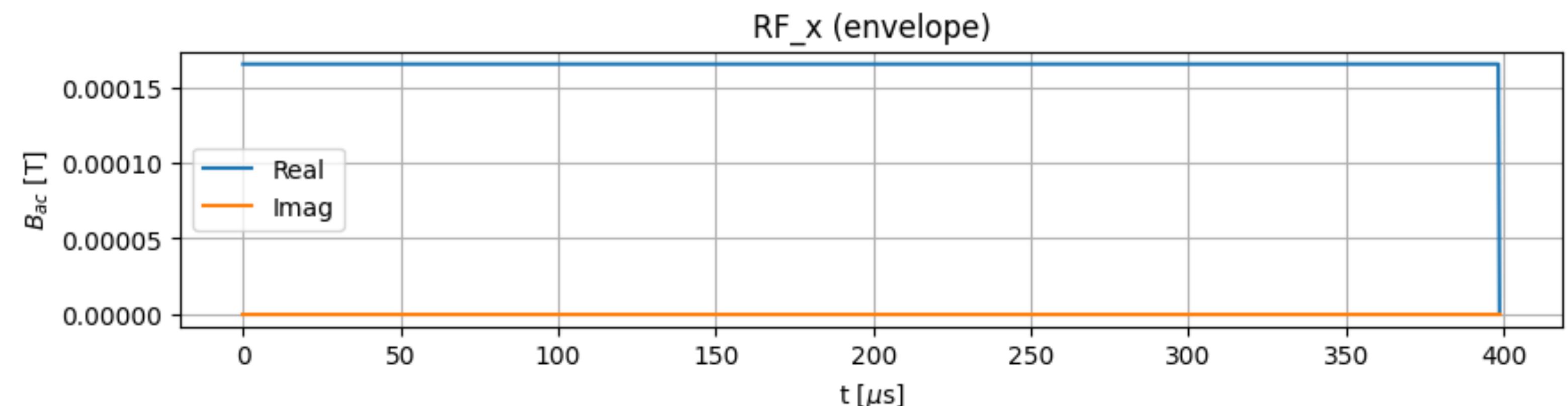
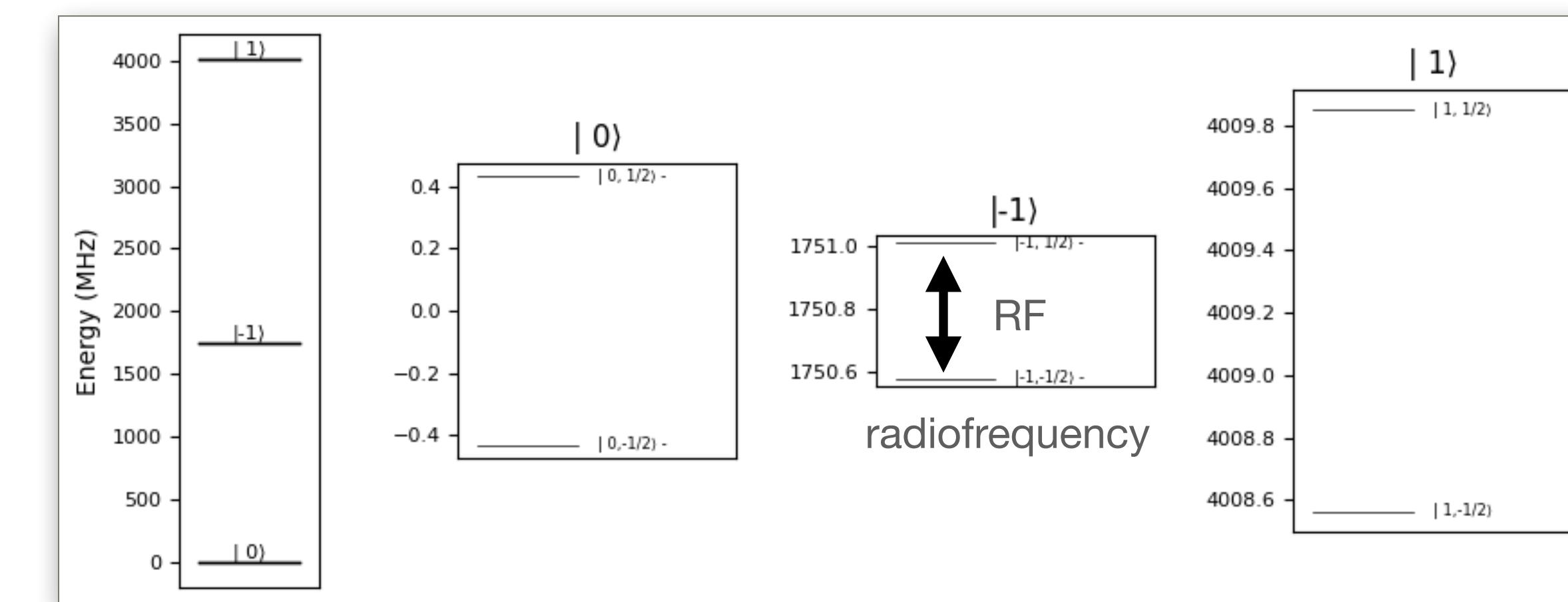


# Multi-spin setup

```
spin_e = simphony.Spin(  
    dimension = 3,  
    name = 'NV-e',  
    gyromagnetic_ratio = 28020, # MHz/T  
    qubit_subspace = (0, -1),  
    zero_field_splitting = 2880 # MHz  
)  
  
spin_C = simphony.Spin(  
    dimension = 2,  
    name = '13C',  
    gyromagnetic_ratio = 10.71, # MHz/T  
    qubit_subspace = (-1/2, 1/2),  
    zero_field_splitting = 0  
)  
  
hyperfine = simphony.Interaction(spin_e, spin_C)  
hyperfine.zz = 0.213154 # MHz  
hyperfine.xz = 0.003 # MHz  
hyperfine.zx = 0.003 # MHz  
  
static_field = simphony.StaticField()  
static_field.z = 0.0403 # T  
  
driving_field_MW = simphony.DrivingField(direction = [1, 0, 0], name = 'MW_x')  
driving_field_RF = simphony.DrivingField(direction = [1, 0, 0], name = 'RF_x')
```

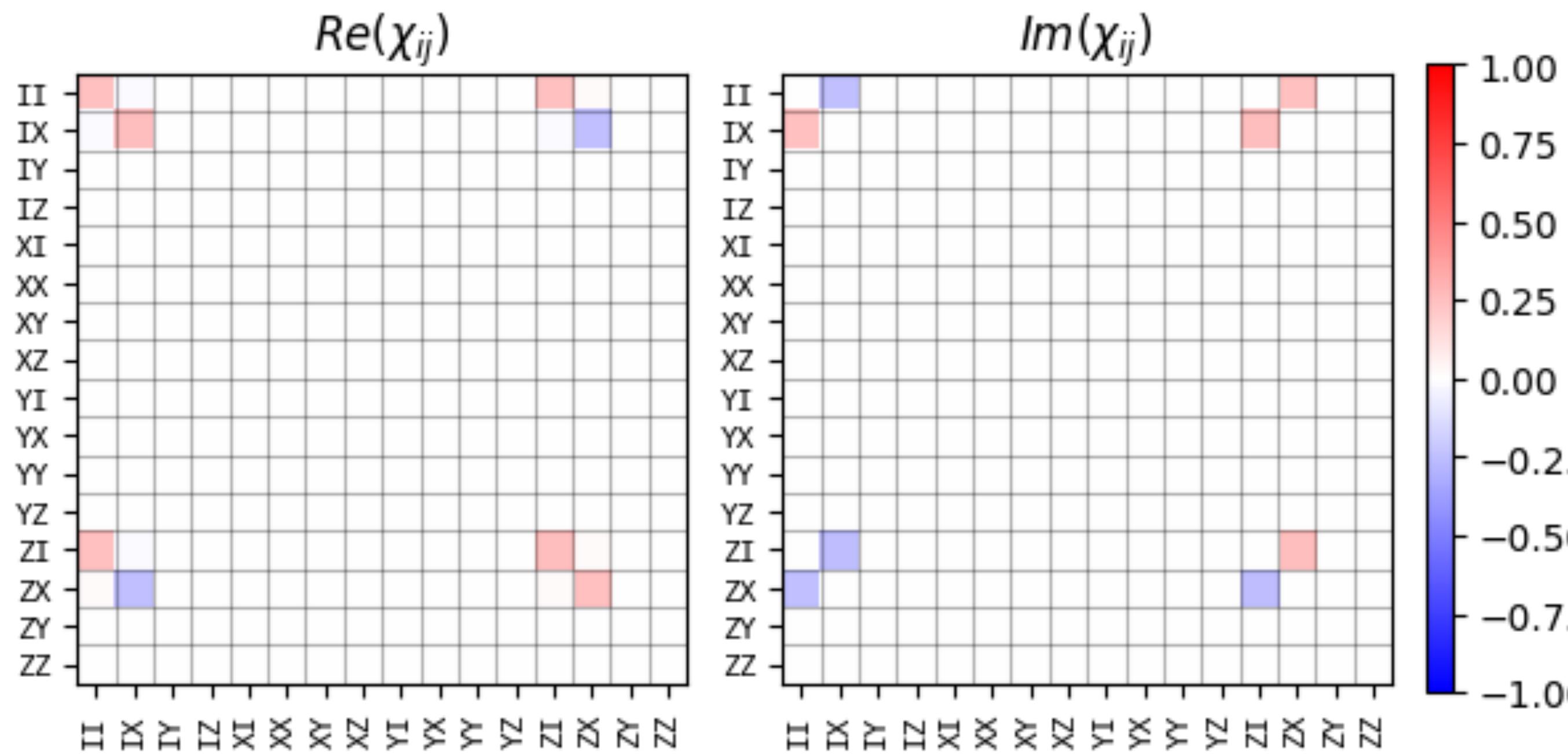


# Conventional nuclear magnetic resonance



# Conventional nuclear magnetic resonance

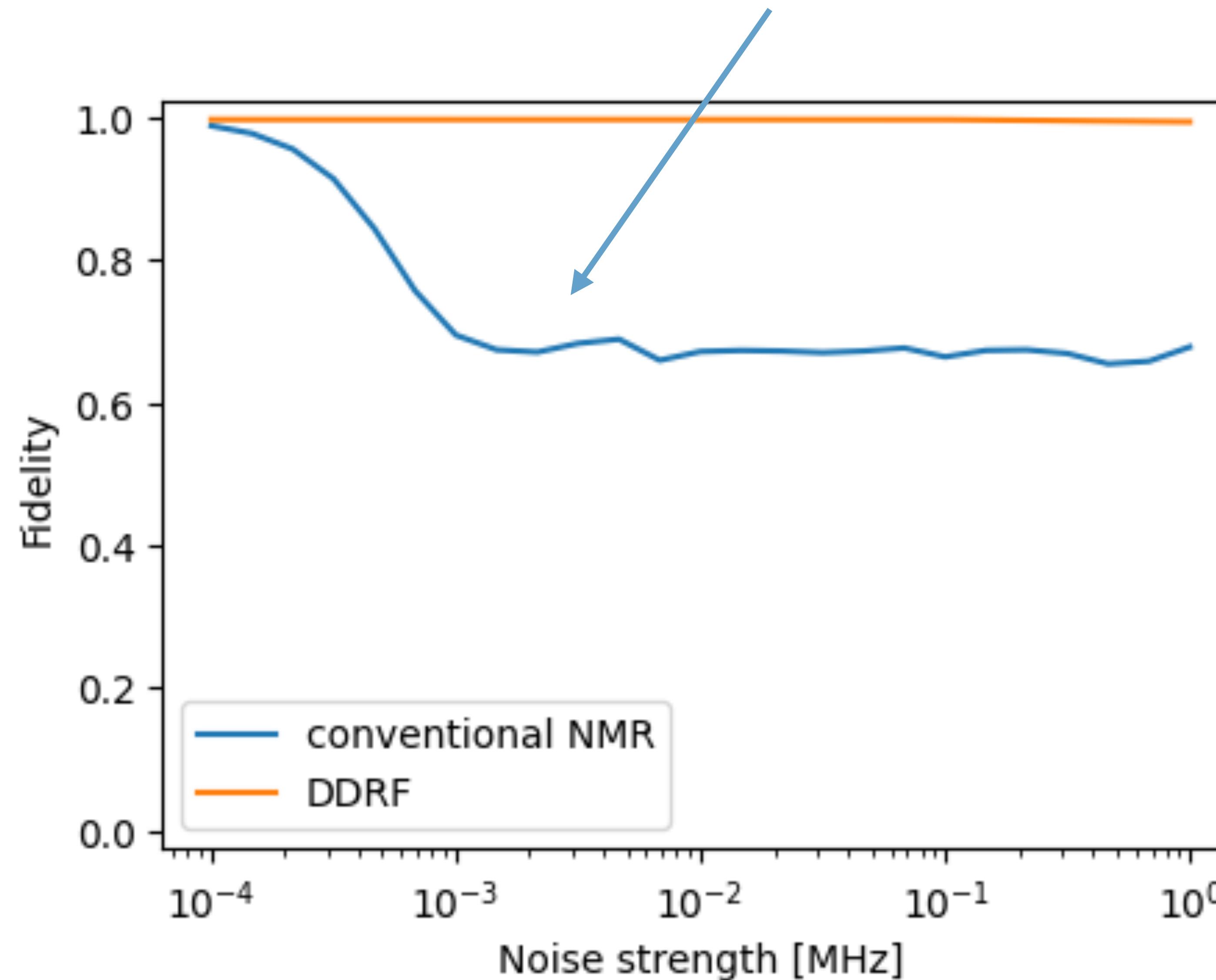
Process matrix



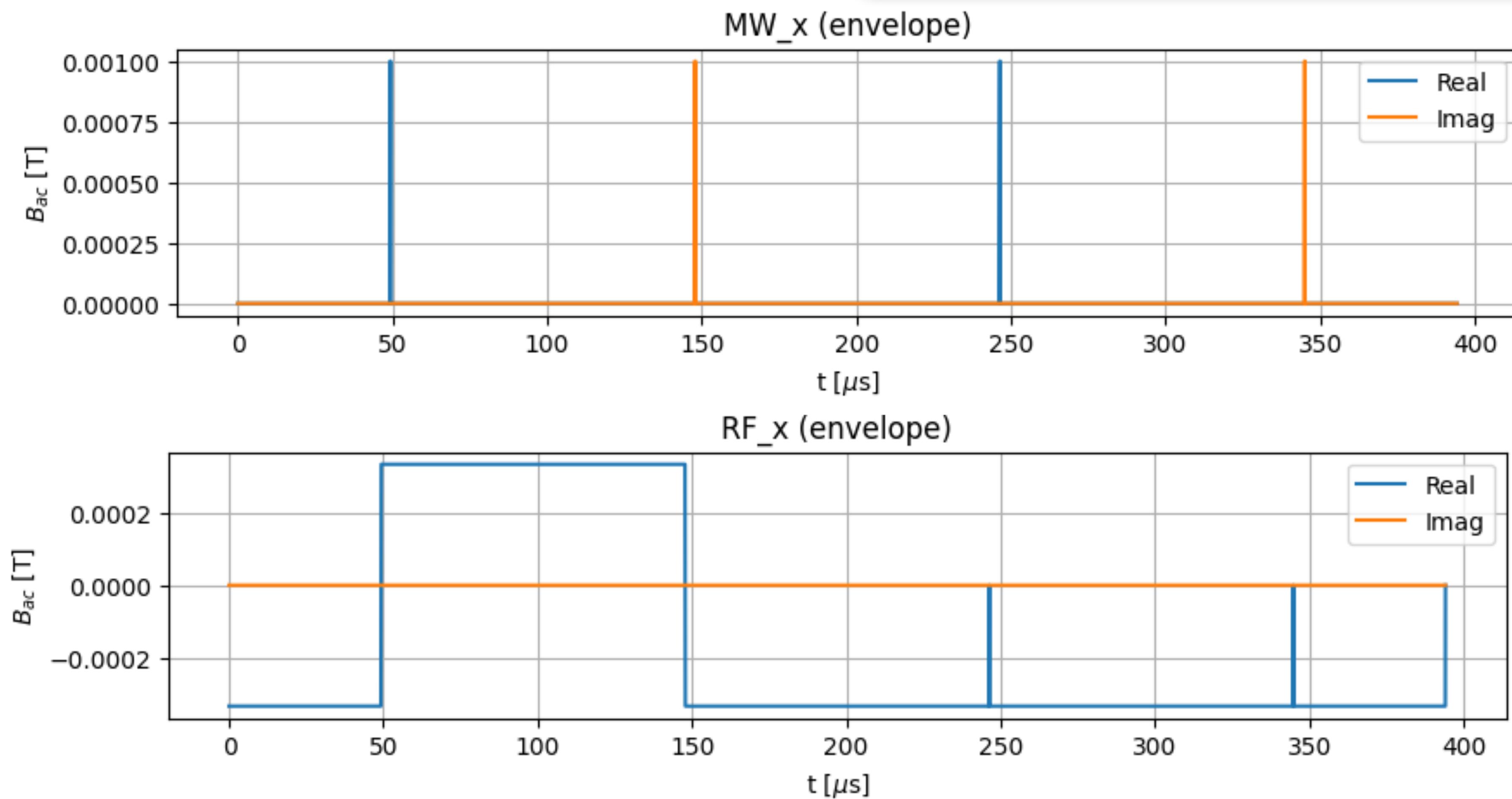
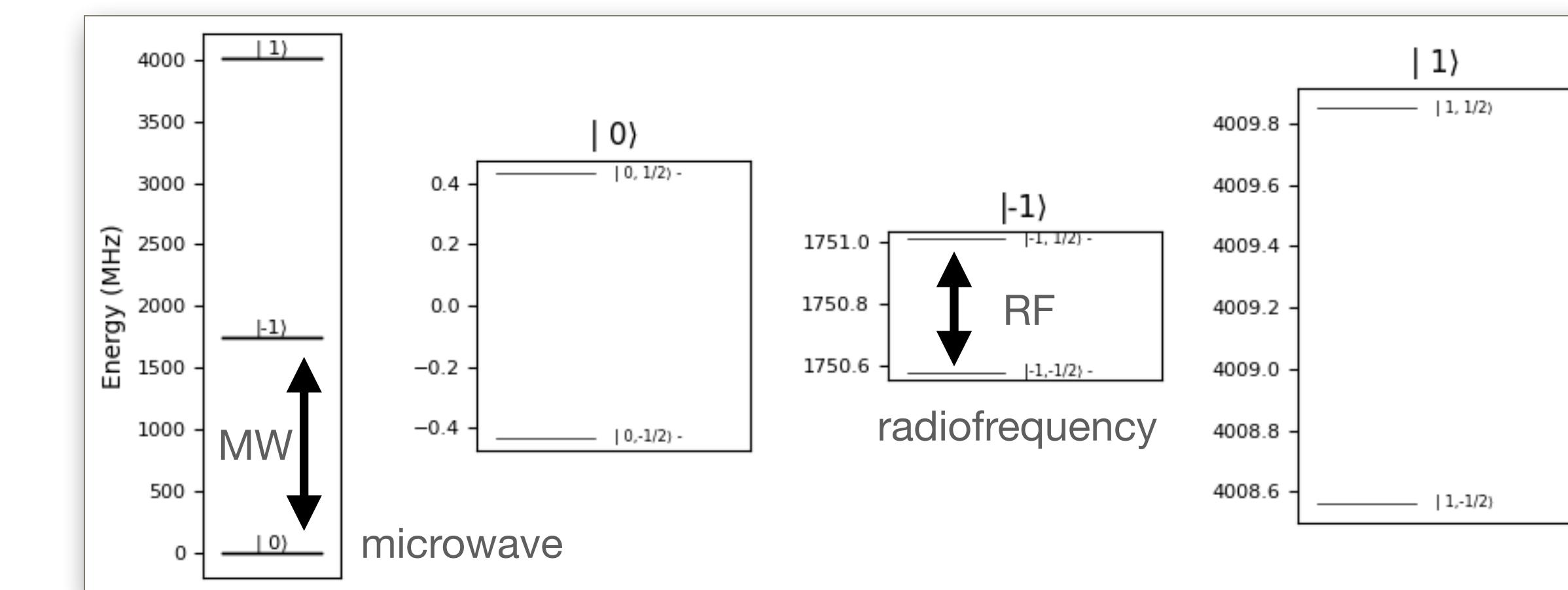
Ideal gate:  
 $RX(\pi)$  controlled on  $m_S = -1$

Average gate fidelity:  
99.87%

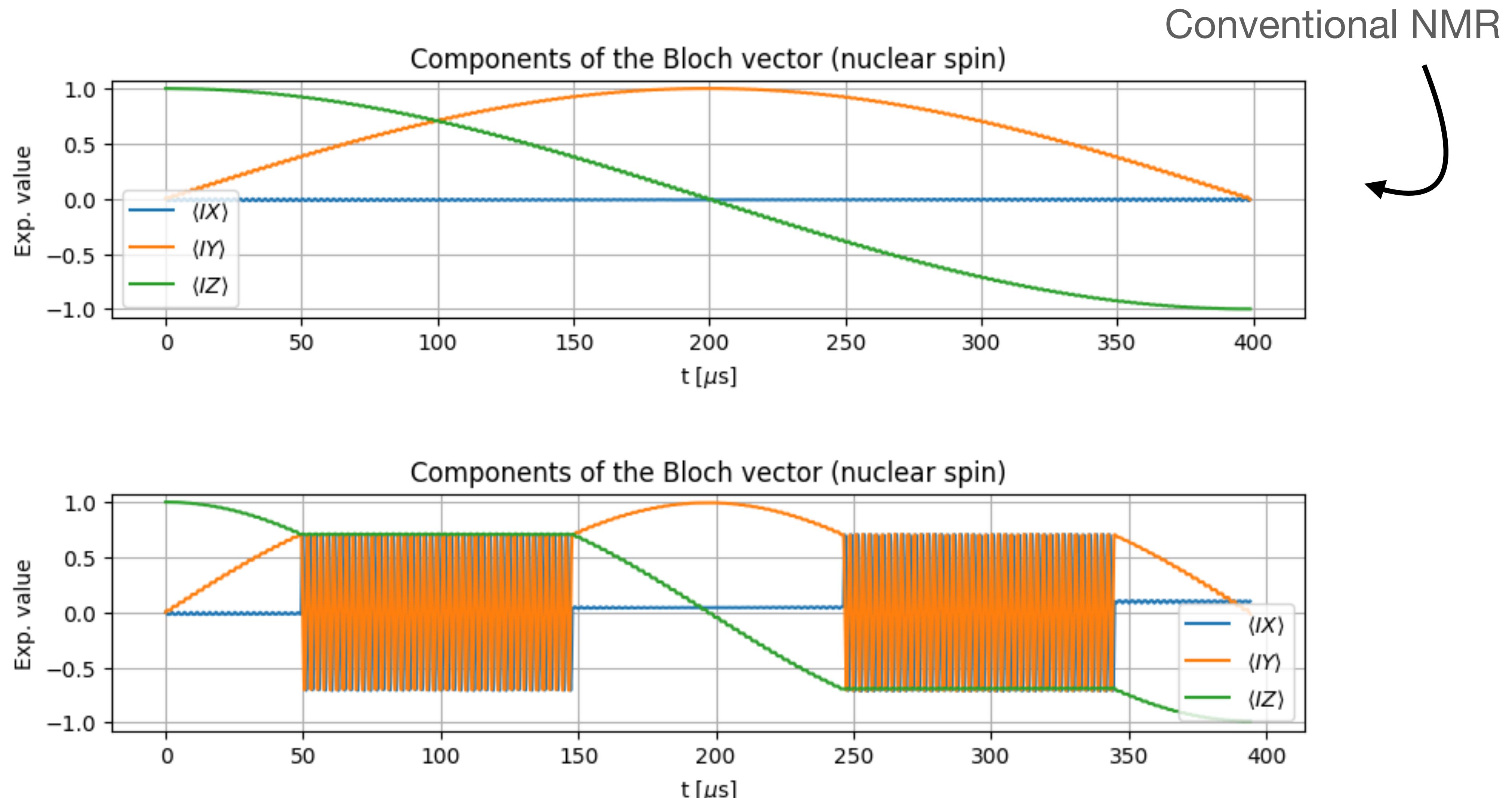
# Conventional NMR: vulnerable to noise



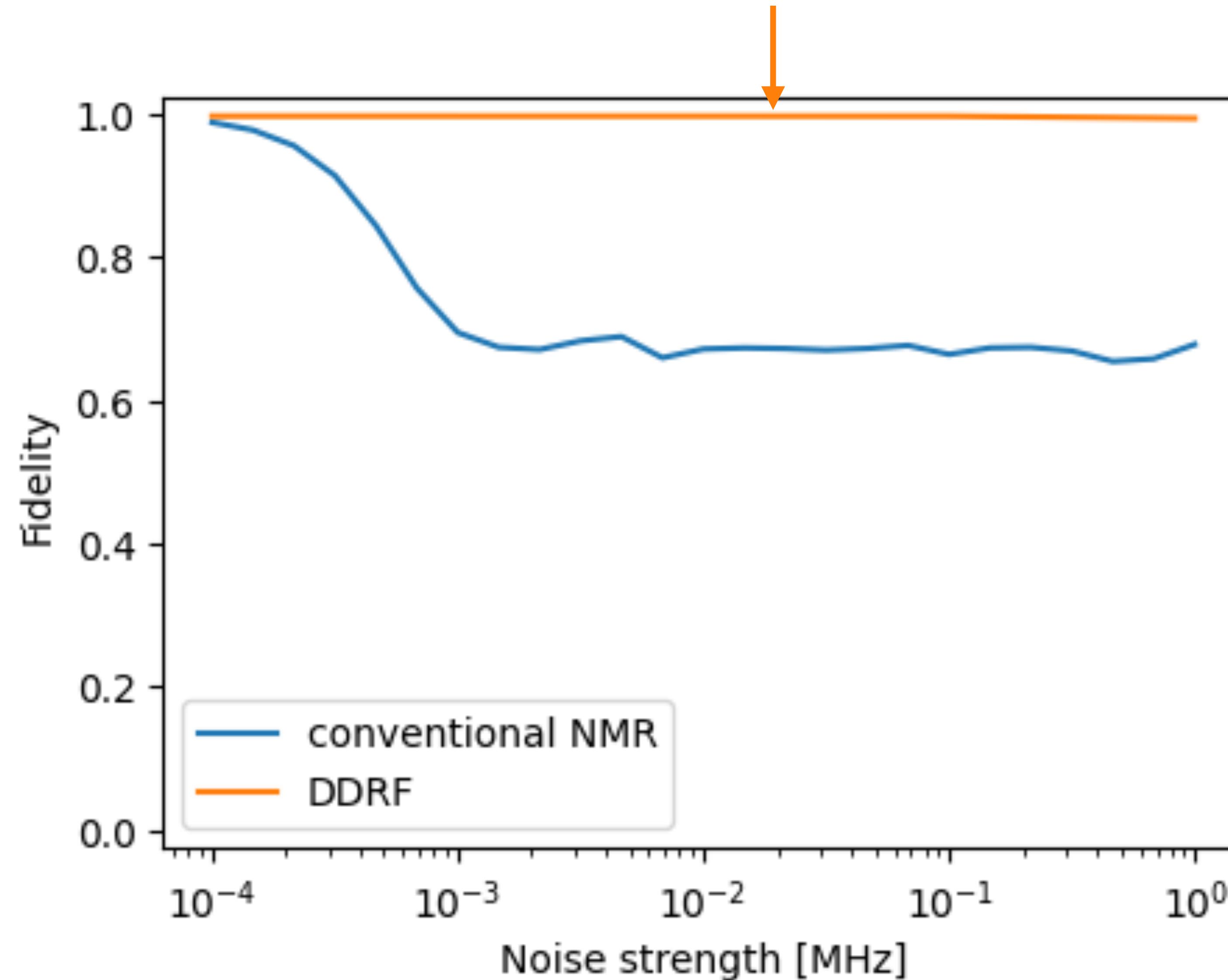
# DDRF pulse sequence



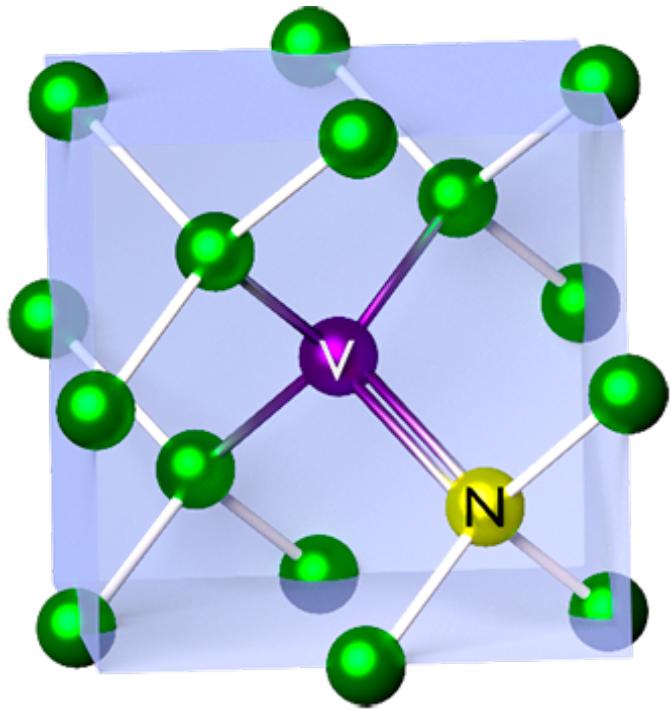
# Spin dynamics due to DDRF pulse sequence



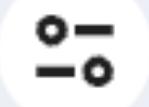
# DDRF pulse sequence: robust against noise



# Simphony



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## Roadmap

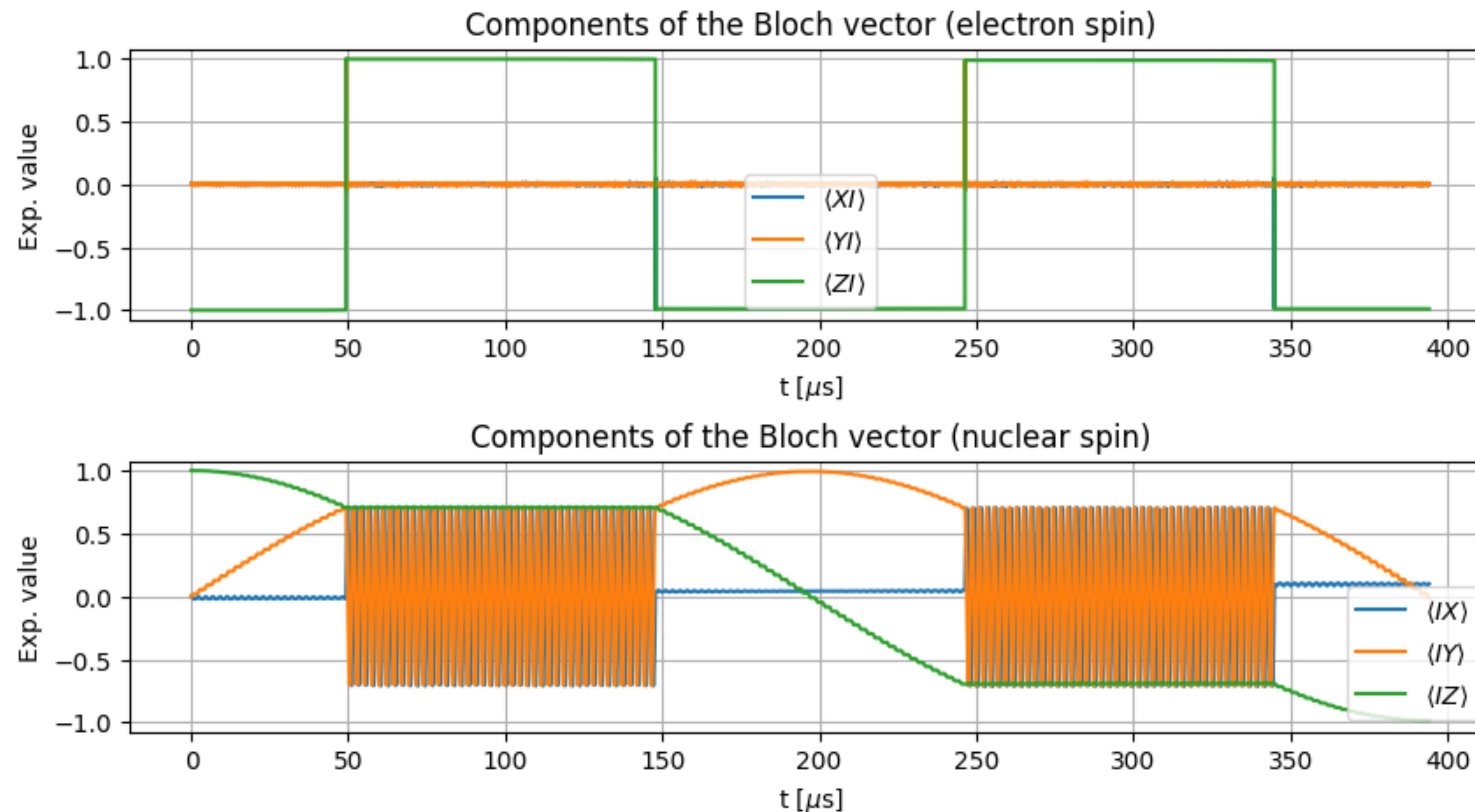
- Integration of <sup>13</sup>C hyperfine database.
- Integration of point-defect Hamiltonians beyond NV centers.
- Scalable registers of coupled NV centers.
- Lindblad-type noise models.
- Non-Markovian system-bath interaction.
- Photophysics dynamics: initialisation and readout.

## Summary

- Simphony is our python package to simulate point defect spin dynamics for quantum technology applications.
- Simphony is our “Minimal Viable Product” => **We are looking for collaborators!**



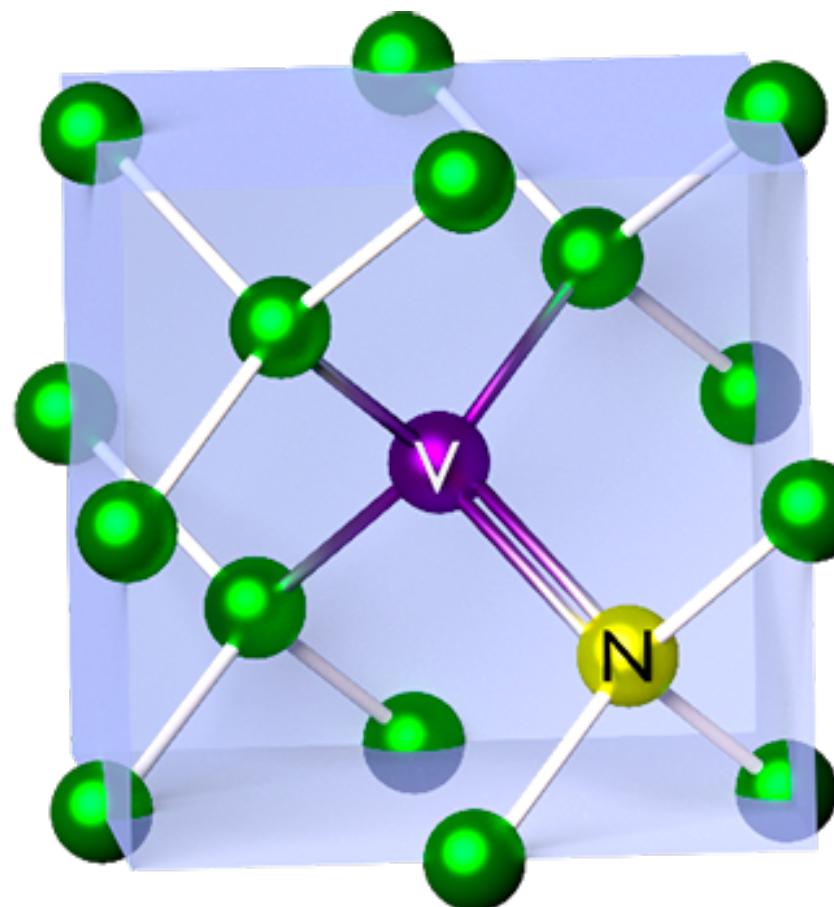
# DDRF pulse sequence



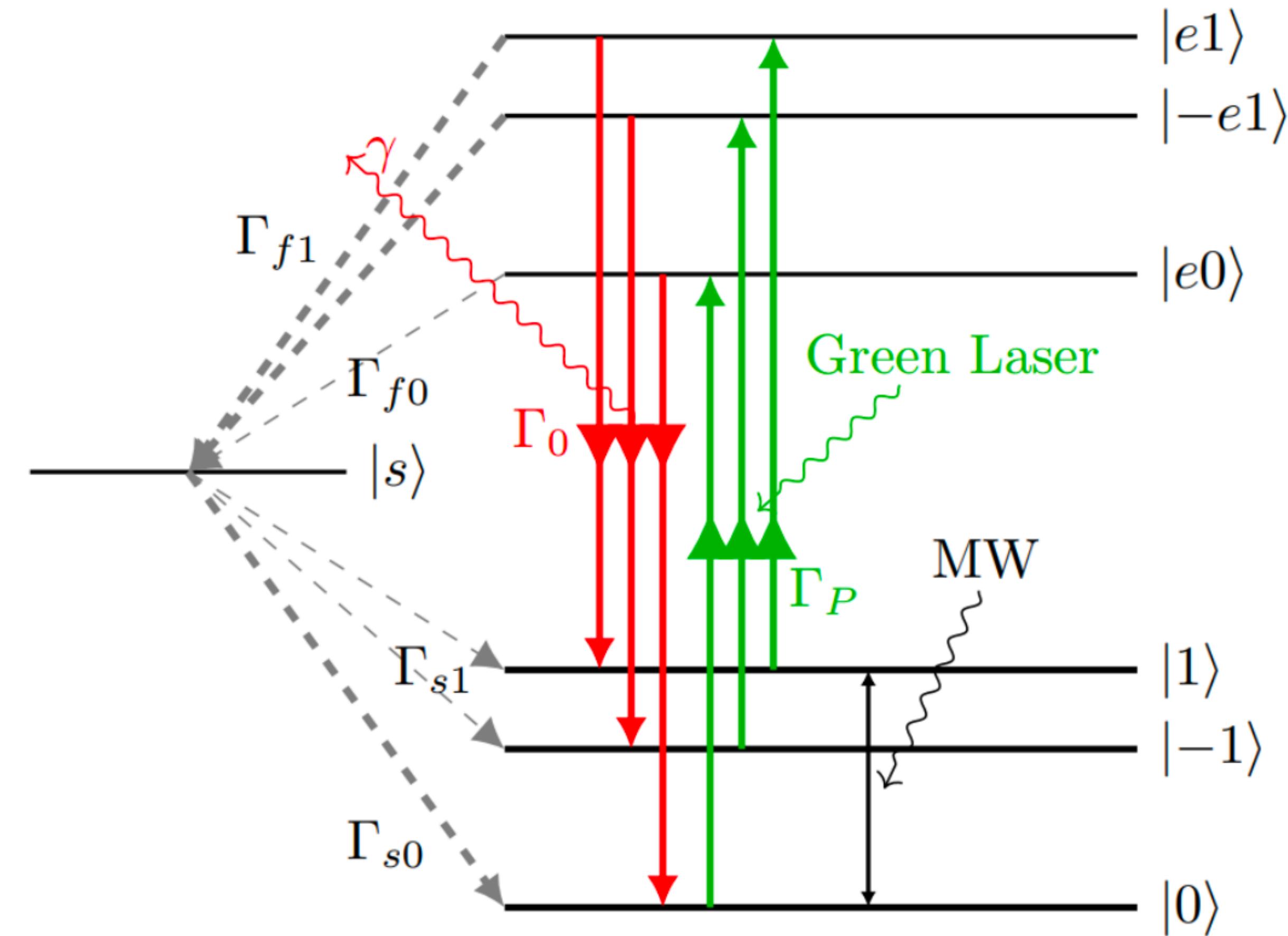
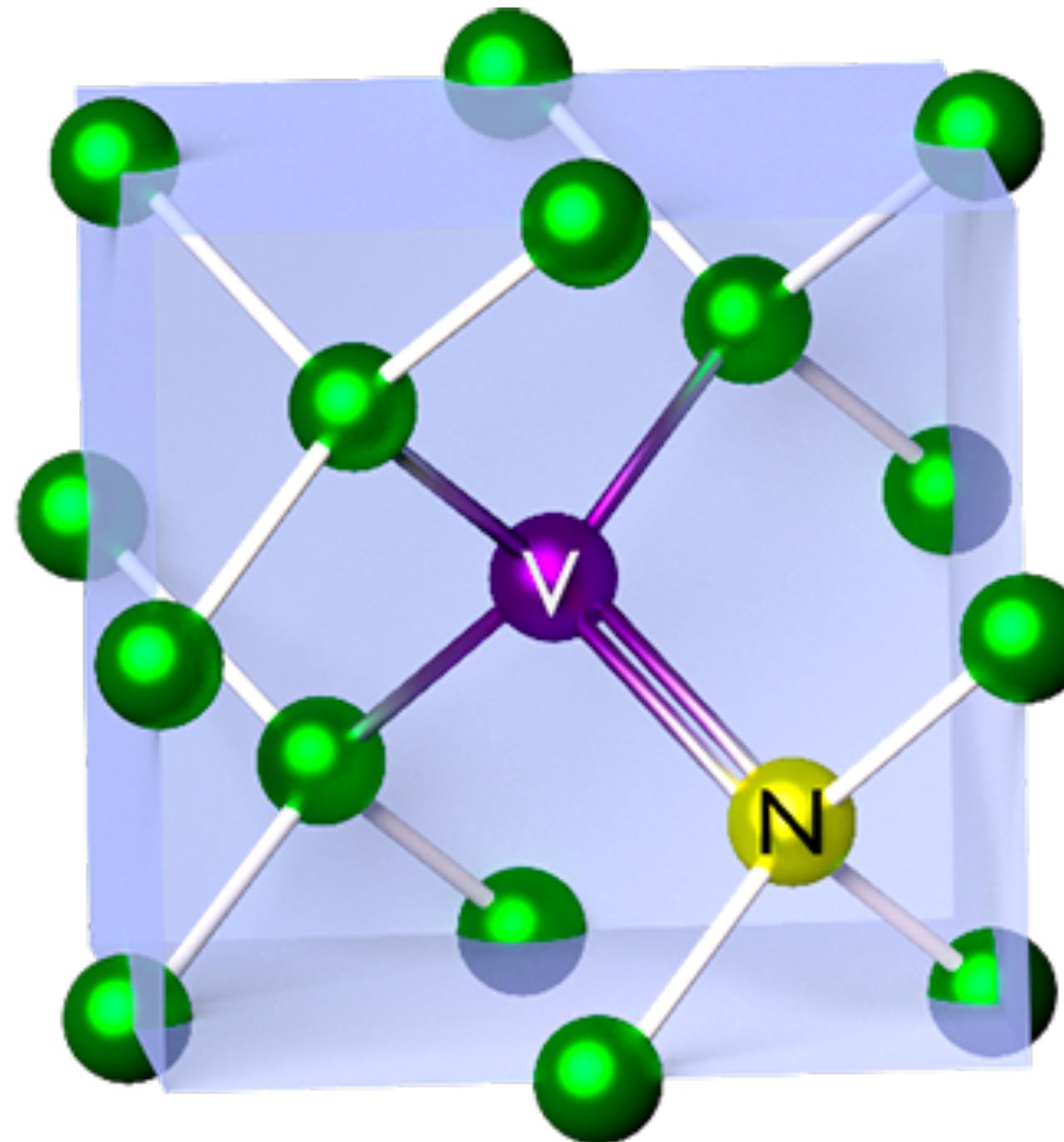
# Towards an AI tool to enhance qubit readout in NV-based registers

## How could this tool improve readout?

- Single-shot readout at elevated temperatures.
- In multi-shot readout (standard for room temperature): reduce the number of shots needed for a given precision.

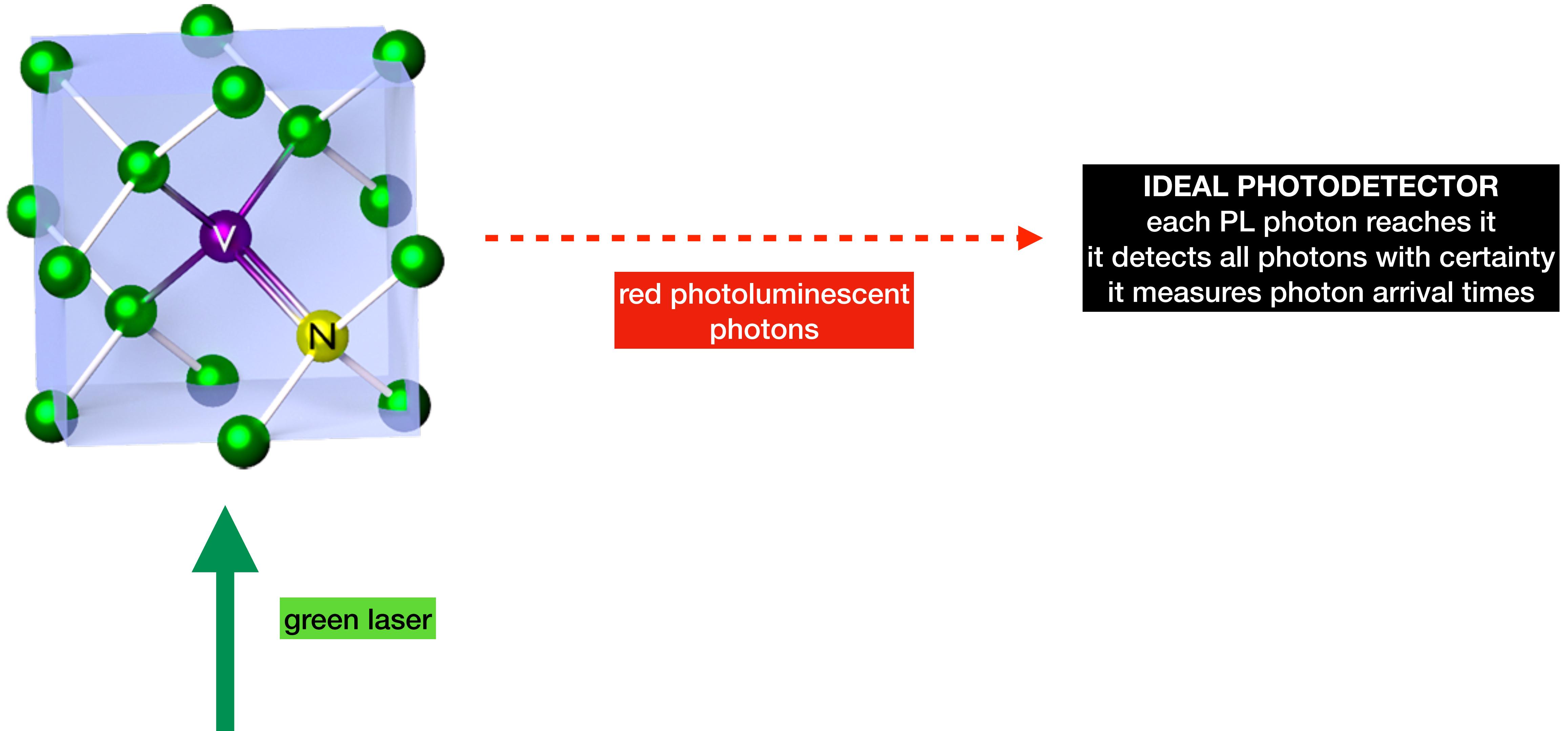


# Towards an AI tool to enhance qubit readout in NV-based registers



ical values of the decay rates are  $\Gamma_0 \simeq 63$  MHz,  $\Gamma_{f0} \simeq 12$  MHz,  $\Gamma_{f1} \simeq 80$  MHz,  $\Gamma_{s1} \simeq 2.4$  MHz and  $\Gamma_{s0} \simeq 3.3$  MHz

# Minimal model to understand fundamental limitations of readout



# Model: photon-number-resolved master equation

$$\dot{\rho}_0^n = -i\frac{\Omega}{2}(\rho_{01}^n - \rho_{10}^n) - \frac{\gamma_1}{2}(\rho_0^n - \rho_1^n) - \frac{\gamma_1}{2}(\rho_0^n - \rho_{-1}^n) - \Gamma_P \rho_0^n + \Gamma_0 \rho_{e0}^{n-1} + \Gamma_{s0} \rho_s^n,$$

$$\dot{\rho}_1^n = i\frac{\Omega}{2}(\rho_{01}^n - \rho_{10}^n) + \frac{\gamma_1}{2}(\rho_0^n - \rho_1^n) - \Gamma_P \rho_1^n + \Gamma_0 \rho_{e1}^{n-1} + \Gamma_{s1} \rho_s^n,$$

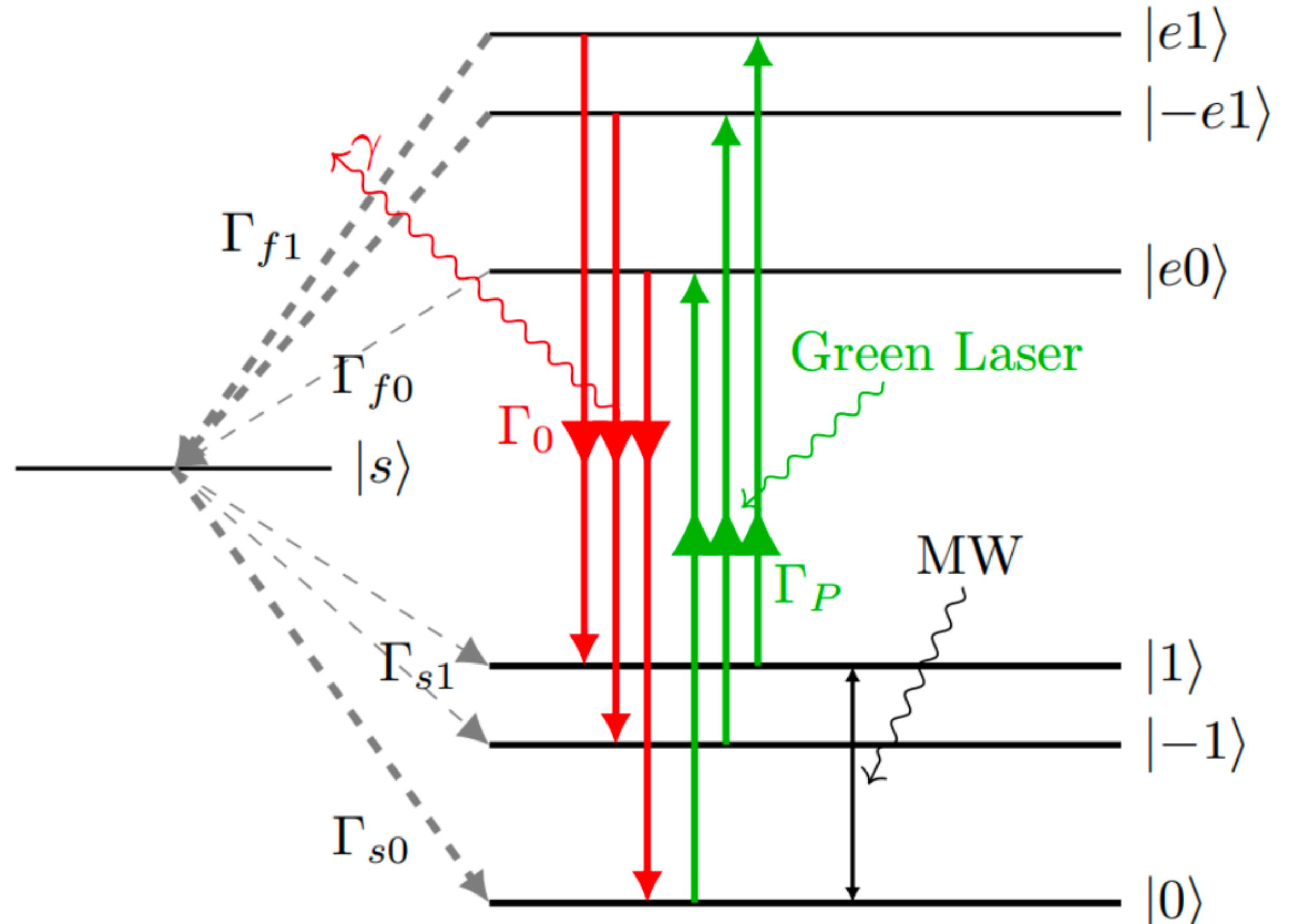
$$\dot{\rho}_{-1}^n = \frac{\gamma_1}{2}(\rho_0^n - \rho_{-1}^n) - \Gamma_P \rho_1^n + \Gamma_0 \rho_{-e1}^{n-1} + \Gamma_{s1} \rho_s^n,$$

$$\dot{\rho}_{e0}^n = \Gamma_P \rho_0^n - \Gamma_0 \rho_{e0}^n - \Gamma_{f0} \rho_{e0}^n,$$

$$\dot{\rho}_{e1}^n = \Gamma_P \rho_1^n - \Gamma_0 \rho_{e1}^n - \Gamma_{f1} \rho_{e1}^n,$$

$$\dot{\rho}_{-e1}^n = \Gamma_P \rho_{-1}^n - \Gamma_0 \rho_{-e1}^n - \Gamma_{f1} \rho_{-e1}^n,$$

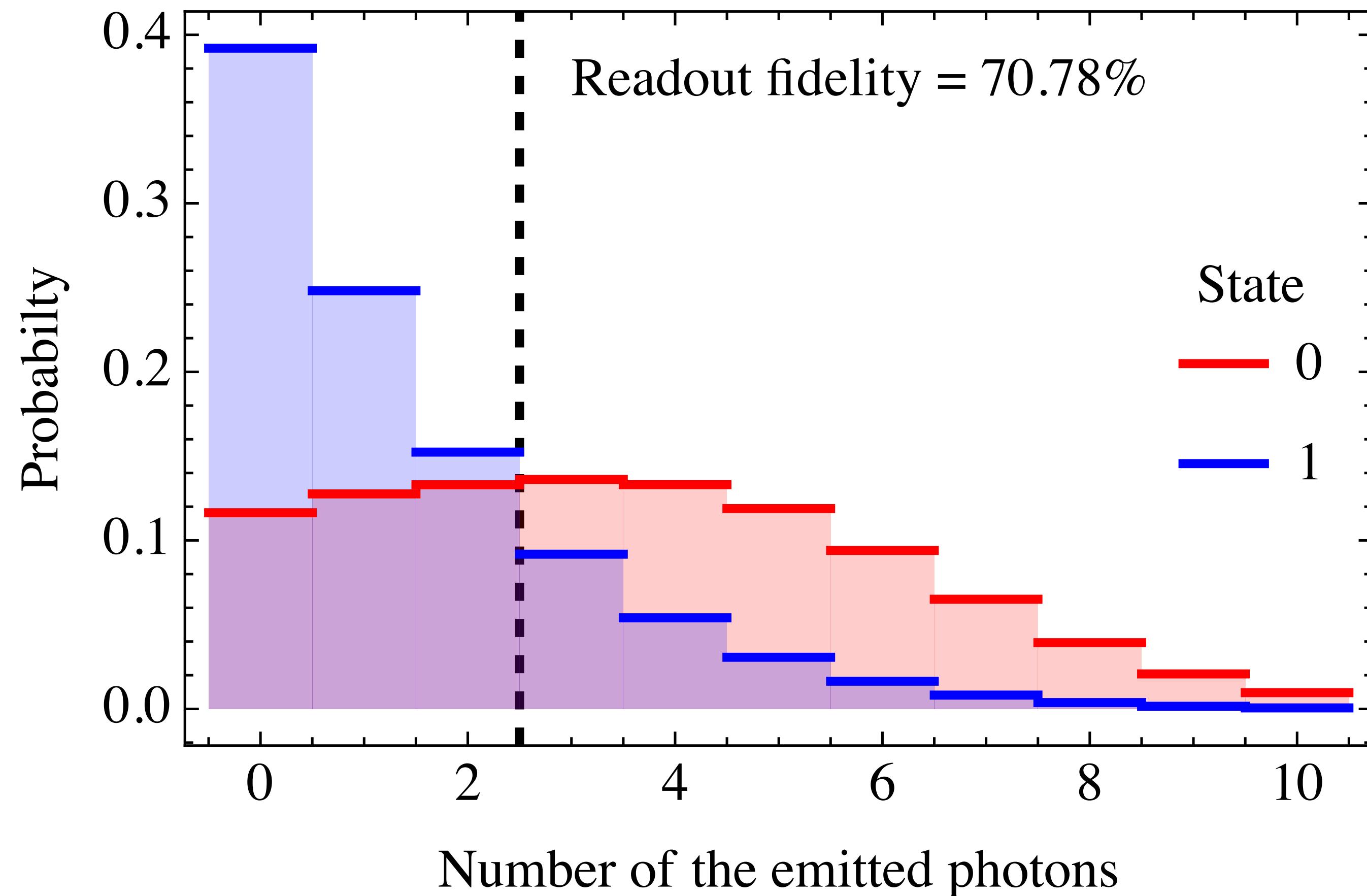
$$\dot{\rho}_s^n = \Gamma_{f1} \rho_{e1}^n + \Gamma_{f1} \rho_{-e1}^n + \Gamma_{f0} \rho_{e0}^n - (\Gamma_{s0} + \Gamma_{s1}) \rho_s^n.$$



ical values of the decay rates are  $\Gamma_0 \simeq 63$  MHz,  $\Gamma_{f0} \simeq 12$  MHz,  $\Gamma_{f1} \simeq 80$  MHz,  $\Gamma_{s1} \simeq 2.4$  MHz and  $\Gamma_{s0} \simeq 3.3$  MHz

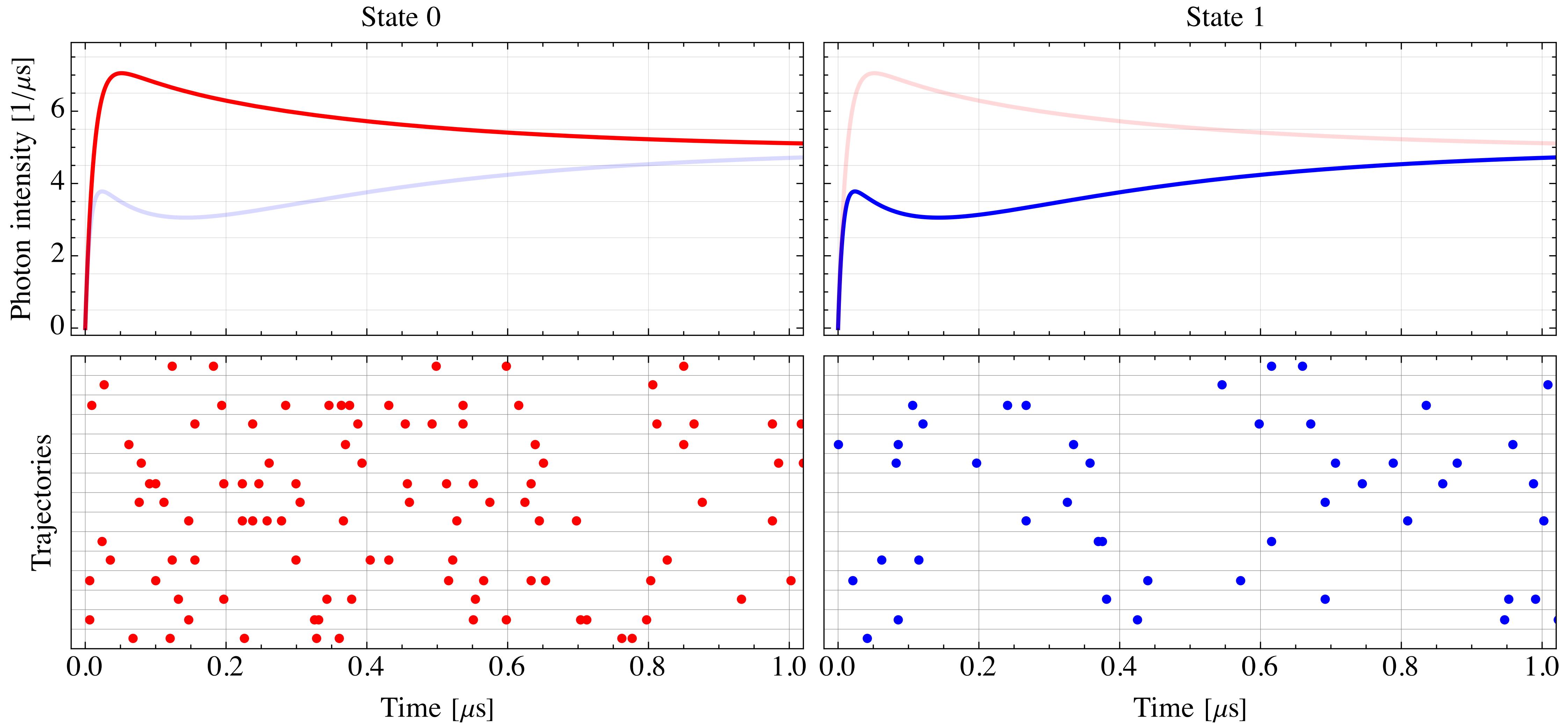
# Photon count reveals partial information about qubit state

- (1) fixed laser intensity
  - (2) fixed 'integration time'
- red/blue:  
photon-count histograms  
for 0/1 qubit basis states



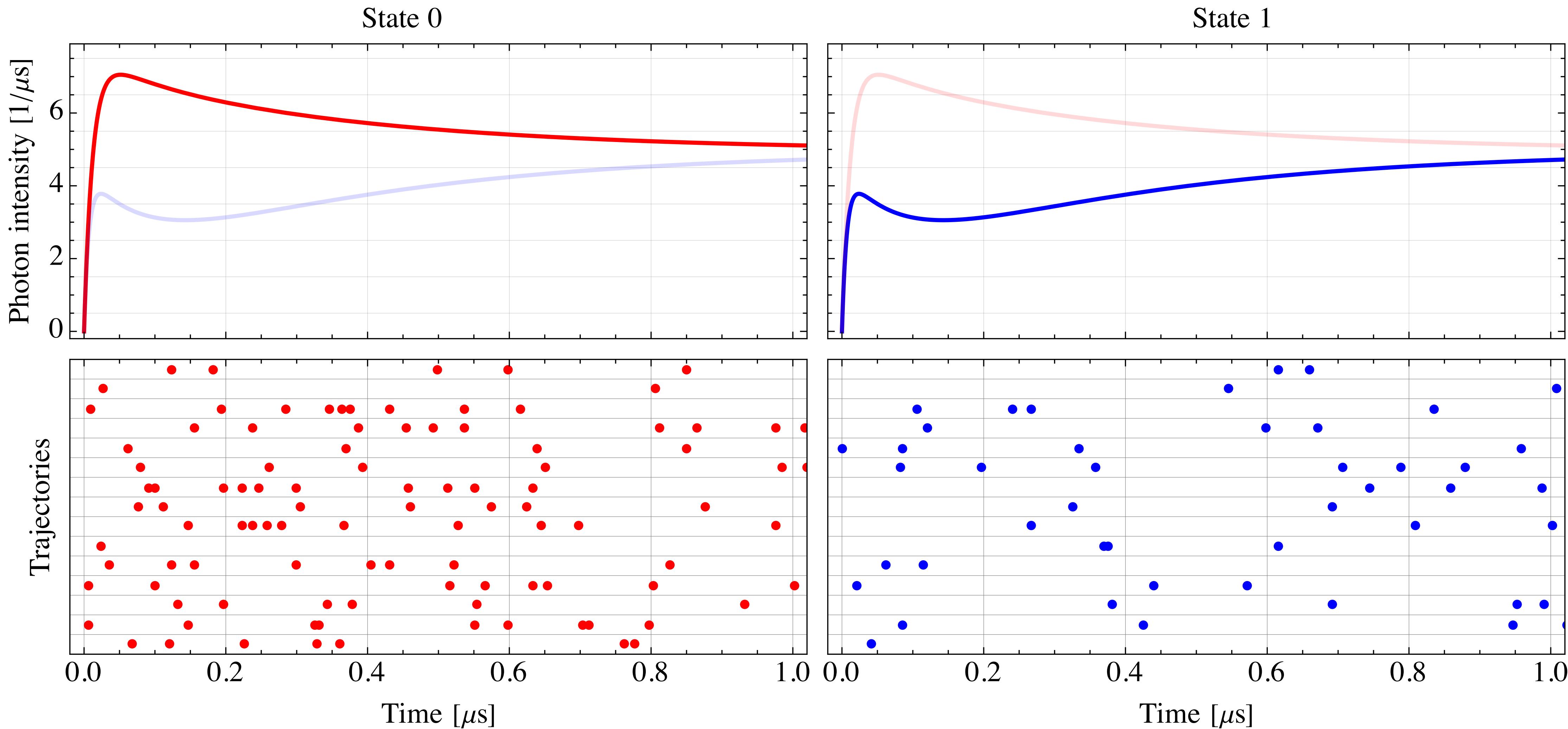
Laser intensity = 10 x PL decay rate.  
Integration time = 0.1 us

# Photon detection trajectories from the master equation



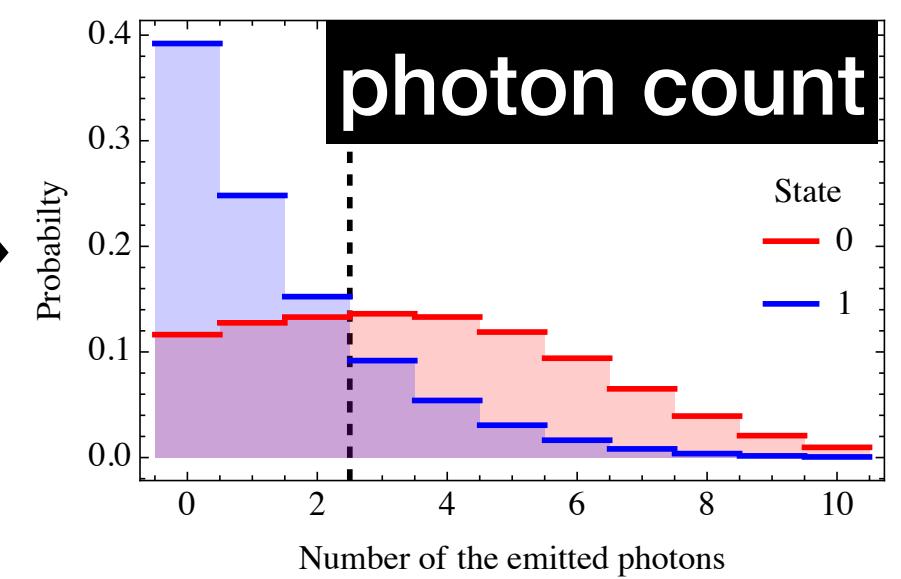
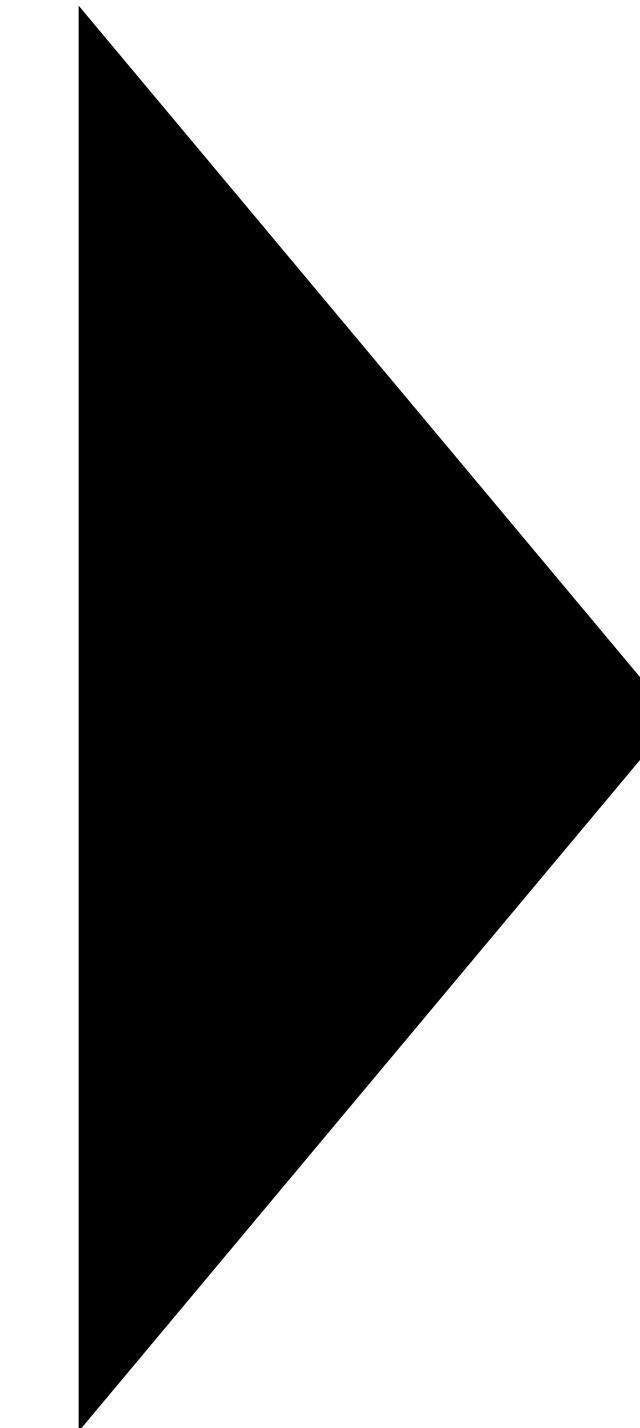
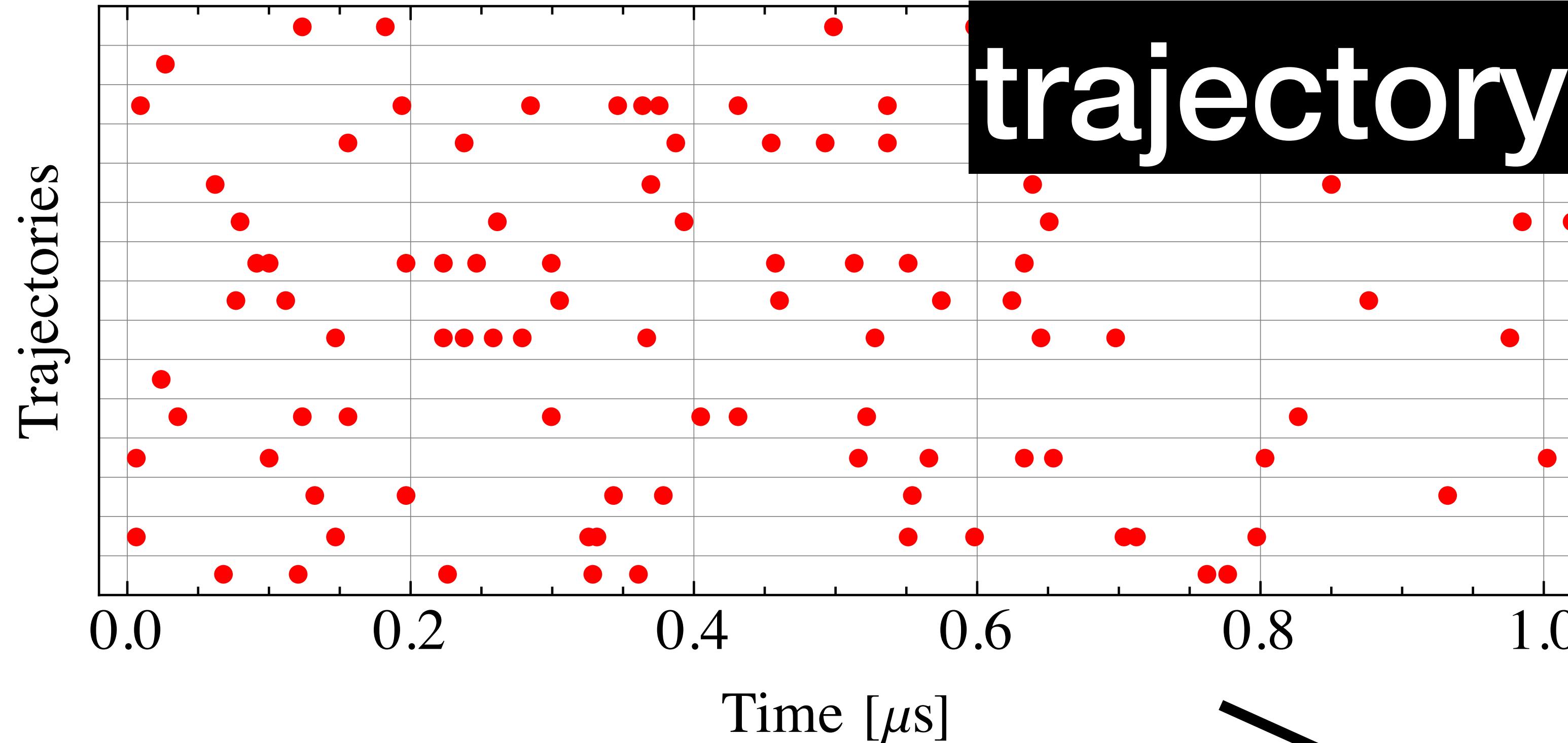
Laser intensity = 0.16 x PL decay rate.

# There is more information in the trajectory than in the photon count!



Laser intensity = 0.16 x PL decay rate.

# There is more information in the trajectory than in the photon count!



We try to squeeze out a more precise qubit readout  
from the more complete information present in the trajectories.

inferred bit, 0 or 1



# Photon count trajectories from master equation

$$\begin{aligned}\dot{\rho}_0^n &= -i\frac{\Omega}{2}(\rho_{01}^n - \rho_{10}^n) - \frac{\gamma_1}{2}(\rho_0^n - \rho_1^n) - \frac{\gamma_1}{2}(\rho_0^n - \rho_{-1}^n) \\ &\quad - \Gamma_P \rho_0^n + \Gamma_0 \rho_{e0}^{n-1} + \Gamma_{s0} \rho_s^n,\end{aligned}$$

$$\begin{aligned}\dot{\rho}_1^n &= i\frac{\Omega}{2}(\rho_{01}^n - \rho_{10}^n) + \frac{\gamma_1}{2}(\rho_0^n - \rho_1^n) \\ &\quad - \Gamma_P \rho_1^n + \Gamma_0 \rho_{e1}^{n-1} + \Gamma_{s1} \rho_s^n,\end{aligned}$$

$$\dot{\rho}_{-1}^n = \frac{\gamma_1}{2}(\rho_0^n - \rho_{-1}^n) - \Gamma_P \rho_1^n + \Gamma_0 \rho_{-e1}^{n-1} + \Gamma_{s1} \rho_s^n,$$

- (1) Given transition rates  $W_{i \leftarrow j}$  and initial time  $t = 0$
- (2) Given state  $j$
- (3) Random realization of the jump times  $\tau_i \sim \text{Exp}(1/W_{i \leftarrow j})$  ( $\forall i$ )
- (4)  $j \leftarrow \text{argmin}_i \tau_i$  is the new state and  $t \leftarrow t + \min \tau_i$
- (5) if  $t > t_{\max}$  break else goto (2)

$$\dot{\rho}_{e0}^n = \Gamma_P \rho_0^n - \Gamma_0 \rho_{e0}^n - \Gamma_{f0} \rho_{e0}^n,$$

$$\dot{\rho}_{e1}^n = \Gamma_P \rho_1^n - \Gamma_0 \rho_{e1}^n - \Gamma_{f1} \rho_{e1}^n,$$

$$\dot{\rho}_{-e1}^n = \Gamma_P \rho_{-1}^n - \Gamma_0 \rho_{-e1}^n - \Gamma_{f1} \rho_{-e1}^n,$$

$$\dot{\rho}_s^n = \Gamma_{f1} \rho_{e1}^n + \Gamma_{f1} \rho_{-e1}^n + \Gamma_{f0} \rho_{e0}^n - (\Gamma_{s0} + \Gamma_{s1}) \rho_s^n.$$

