Pymond: a package for system-level simulation of solid-state based quantum technologies

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The estimation of the performance of solid-state-defect-based quantum devices [1] lacks a system-level approach beyond the performance of an ideal single point. In this work we present the python package *pymond*, aimed at bridging the gap between theoretical and experimentally realistic estimates of performance [2][3]. We prioritize a systematically semi-analytical approximation, widely valid under typical conditions in quantum control, which in turn provides high-speed simulation capabilities as compared to heavily numerical tools [4]. This enables system-level optimization of quantum control protocols and device design, essential from academic to industrial applications.

The package has initially been developed for the optimization of the performance of quantum sensors using nitrogen-vacancy (NV) centres in diamond but features a modular structure allowing straightforward extension to other solid-state-defect-based technologies.

References

[1] Thiering et al., Semiconductors and Semimetals, 103 (2020), 1-36
[2] Barry et al., Reviews of Modern Physics, 92 (2020), 015004
[3] Jarmola et al., Science Advances, 7 (2021), eabl3840
[4] Johansson et al., Computer Physics Communications, 183 (2012), 1760

Figures

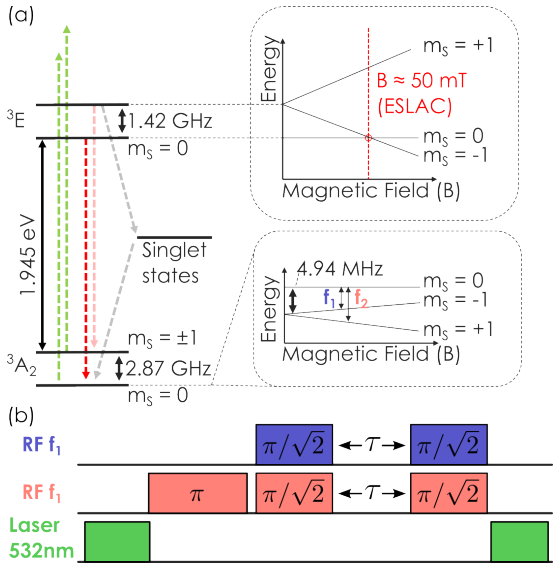

Figure 1: (a) Modelled energy-level structure of the NV- at excited state level anti-crossing (ESLAC), for which *pymond* can simulate full-device optical spin polarization-readout and quantum control schemes, such as (b) nuclear Double Quantum (DQ) Ramsey.

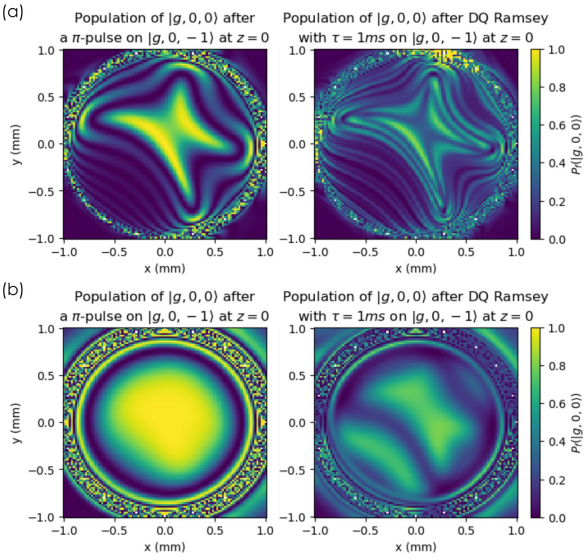

Figure 2: Population of the $|g, 0, 0\rangle$ state of NV- after a π-pulse (left) and DQ Ramsey sequence (right) on $|g, 0, -1\rangle$ for an inhomogeneous magnetic field and a ⌀=1mm antenna with peak currents of (a) I=0.1A and (b) I=1A.