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RydIQule Version 2: Enhancing graph-based modeling of Rydberg atoms

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Summary

Rydberg atomic radio-frequency (rf) sensors are an emerging technology platform that relies on vaporous atoms, interrogated with laser beams and nearly ionized, to receive rf signals. Rydberg rf sensors have a number of interesting fundamental distinctions from traditional receiver technologies, such as those based on metallic antennas, since they are governed by the quantum physics of atom-light interactions (Fancher et al., 2021). As Rydberg sensors quickly advance from laboratory experiments into fieldable devices, there is a need for a general software modeling tool that fully encompasses the internal physics of the sensor. The Rydberg Interactive Quantum Module (RydIQule) is a Python package designed to fill this need.

RydIQule calculates the dynamics of atomic quantum states, with a particular emphasis on modeling thermal vapors of Rydberg atoms coupled to optical and radio-frequency electromagnetic fields. To accomplish this, a unique graph-based paradigm is used to represent the complex quantum system consisting of multiple energy levels and multiple electromagnetic fields, where each energy level is stored as a graph node and each electromagnetic coupling as a graph edge. RydIQule then generates a set of differential equations for the quantum state dynamics from the graph, using the Lindblad master equation formalism (Manzano, 2020). Finally, RydIQule leverages linear equation solvers, such as those provided by NumPy (Harris et al., 2020), SciPy (Virtanen et al., 2020) or CyRK (Renaud, 2022) to efficiently solve these systems and recover the quantum system response to arbitrary input fields. During the numerical solving, systems of equations are represented as tensor objects, allowing for efficient parameterization and computation of large sets of equations. All together, RydIQule provides a flexible platform for forward modeling Rydberg sensors while also providing a widely useful set of theoretical tools for fundamental exploration of atomic physics concepts.

The initial public release of RydIQule in late 2023 built the core functionality described above (Miller et al., 2024). Here we outline RydIQule's version 2 release which expands on its capabilities to more accurately model real-world atoms.

Statement of Need

The unique quantum properties of Rydberg atoms offer distinct advantages in the fields of sensing, communication, and quantum information (Adams et al., 2019). However, the breadth of possible configurations and experimental parameters makes general modeling of an experiment difficult. One challenge is that many atomic energy levels consist of numerous magnetic sublevels that arise from the different possible orientations of the electron's and

nucleus's angular momentum. These sublevels have different responses to applied magnetic and electric fields which leads to measureable differences for most real-world atomic sensors. In some cases, this sublevel structure can be treated in average and safely ignored. More often however, they are ignored due to the significant complexity inherent in expanding the model size to account for them.

For example, in accounting for magnetic splitting, a typical Rydberg spectroscopy experiment using the $5S_{1/2} \rightarrow 5P_{3/2} \rightarrow n$D set of transitions would have a total of 46 levels with up to 34 dipole-allowed couplings between them. In RydIQule's initial release, users would have no choice but to individually add each sublevel and the many associated electromagnetic couplings, making it of little functional use. For this reason, RydIQule was not easily scaled to realistic scenarios involving several atomic states and typically many tens, or possibly even hundreds, of sublevels.

The main advance of RydIQule version 2 is to allow user-friendly inclusion of large atomic manifolds that include the complete set of electronic and magnetic sublevels. In particular, this release introduces a new paradigm for structured labeling of states using arbitrary tuples, and expands the automated calculation of relevant atomic properties on alkali atoms commonly used in Rydberg physics to include sublevels. This release also includes a new steady-state Doppler-averaging method that greatly improves speed and accuracy, along with many other optimizations and improvements to the code-base.

Handling Sublevel Structure

RydIQule's primary improvement in version 2 is in handling state manifolds: degenerate sets of sublevel states defined by a magnetic interaction with the electron. It handles this sublevel structure by expanding the way nodes are labelled. Rather than only using integers, arbitrary tuples can now be used as graph nodes. This allows for manifolds to be defined by using tuples in a way that directly maps to the atomic structure. RydIQule's core functions relating to graph operations have been updated to interchangeably address individual states or entire manifolds. It's internals have been overhauled to not only ensure that all relevant states/couplings are added, but tracked as originating from a single manifold.

Improved Calculation of Atomic Properties

Version 2 of RydIQule also completely overhauls the `Cell` class, which provides automatic calculation of atomic properties of alkali atoms using the Alkali.ne Rydberg Calculator (ARC) package (Robertson et al., 2021; Šibalić et al., 2017). In version 1, this class could only handle simplified atomic models that treated manifolds of atomic sublevels as a single approximate state. Though this type of model is very fast and can be effective in many situations, it breaks down for systems in the presence of magnetic fields (including those as weak as Earth's background magnetic field) or for large electric field amplitudes that result in inhomogeneous couplings due to sublevel structure. By leveraging the tuple labelling outlined above, `Cell` can now define states by their quantum numbers directly, which allows for natural definition and coupling of entire manifolds.

Version 2 also greatly enhances the leveraging of ARC to calculate more system parameters automatically. In particular, there is automatic calculation of coupling strengths between manifolds defined in incommensurate fine and hyperfine bases. This feature allows for more efficient modeling of Rydberg atoms since low energy and high energy states can be defined in their natural bases, fine and hyperfine respectively, lowering the total number of sublevels that need to be calculated.

Analytic Doppler Averaging

Support for steady-state Doppler-averaged models leveraging an exact analytic method has been added. This functionality is based on the theoretical work presented in (Nagib & Walker,

2025). That work derives the exact velocity dependence due to Doppler shifts for a system along a single axis. It effectively reduces the Doppler-averaging integration along that single dimension to two diagonalizations, avoiding velocity sampling that dimension, and enabling a general, analytic result. For example, a two-dimensional Doppler-average only needs to be numerically sampled along one axis, with the other performed analytically. This reduction in dimensionality results in over an order of magnitude reduction in calculation time and memory footprint while returning significantly higher accuracy solutions. Experimental support for 1D solves only was released in version 2.0.0, with RydIQule v2.1.0 providing full support.

Related Packages and Work

Modeling quantum systems using the semi-classical Lindblad formalism is a common task that has been implemented by many physicists for their bespoke problems. Other tools that implement this type of simulation for specific types of problems include: qubits in QuTiP (Johansson et al., 2013), atomic magnetometers in ElecSus (Keaveney et al., 2018), and laser cooling in PyLCP (Eckel et al., 2020). Ultimately, the goal of RydIQule has not been to develop a new modeling technique, but rather to make a common, flexible, and most importantly efficient tool that solves a ubiquitous problem.

RydIQule's version 2 release aims to capture the functionality of the Atomic Density Matrix (ADM) package (Rochester, 2008) written in Mathematica. While very capable, it is built on a proprietary platform requiring a paid license which limits its accessibility. And since Mathematica is an interpreted language, it can lack the speed that compiled libraries like NumPy enable, especially when exploring a large parameter space.

Since RydIQule version 1 has been publicly released, it has been used in several publications to model both general Rydberg atom physics (Backes et al., 2024; Glick et al., 2025; Su et al., 2024) as well as Rydberg sensor development (Cui et al., 2025; Elgee et al., 2023; Gokhale et al., 2024; Richardson et al., 2023; Santamaria-Botello et al., 2022).

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Adams, C. S., Pritchard, J. D., & Shaffer, J. P. (2019). Rydberg atom quantum technologies. *Journal of Physics B: Atomic, Molecular and Optical Physics*, *53*(1), 012002. https://doi.org/10.1088/1361-6455/ab52ef

Backes, K. M., Elgee, P. K., LeBlanc, K.-J., Fancher, C. T., Meyer, D. H., Kunz, P. D., Malvania, N., Nicolich, K. L., Hill, J. C., Marlow, B. L. S., & Cox, K. C. (2024). Performance of antenna-based and Rydberg quantum RF sensors in the electrically small regime. *Applied Physics Letters*, *125*(14), 144002. https://doi.org/10.1063/5.0222827

Cui, M., Zeng, Q., Wang, Z., & Huang, K. (2025). *Realizing quantum wireless sensing without extra reference sources: Architecture, algorithm, and sensitivity maximization*. https://arxiv.org/abs/2504.21234

Eckel, S., Barker, D. S., Norrgard, E. B., & Scherschligt, J. (2020). *PyLCP: A python package for computing laser cooling physics* (No. arXiv:2011.07979). arXiv. https://doi.org/10.48550/arXiv.2011.07979

Elgee, P. K., Hill, J. C., LeBlanc, K.-J. E., Ko, G. D., Kunz, P. D., Meyer, D. H., & Cox, K. C. (2023). Satellite radio detection via dual-microwave Rydberg spectroscopy. *Applied Physics Letters*, *123*(8), 084001. https://doi.org/10.1063/5.0158150

Fancher, C. T., Scherer, D. R., John, M. C. St., & Marlow, B. L. S. (2021). Rydberg Atom Electric Field Sensors for Communications and Sensing. *IEEE Transactions on Quantum Engineering*, *2*, 1–13. https://doi.org/10.1109/TQE.2021.3065227

Glick, J., Anderson, B. E., Nunley, T. N., Bingaman, J., Liu, J. J., Meyer, D. H., & Kunz, P. D. (2025). *Warm vapor rydberg EIT spectra in doppler-free configurations*. https://arxiv.org/abs/2506.04504

Gokhale, P., Carnahan, C., Clark, W., & Chong, F. T. (2024). *Deep Learning for Low-Latency, Quantum-Ready RF Sensing* (No. arXiv:2404.17962). arXiv. https://doi.org/10.48550/arXiv.2404.17962

Harris, C. R., Millman, K. J., van der Walt, S. J., Gommers, R., Virtanen, P., Cournapeau, D., Wieser, E., Taylor, J., Berg, S., Smith, N. J., Kern, R., Picus, M., Hoyer, S., van Kerkwijk, M. H., Brett, M., Haldane, A., del Río, J. F., Wiebe, M., Peterson, P., … Oliphant, T. E. (2020). Array programming with NumPy. *Nature*, *585*(7825), 357–362. https://doi.org/10.1038/s41586-020-2649-2

Johansson, J. R., Nation, P. D., & Nori, F. (2013). QuTiP 2: A Python framework for the dynamics of open quantum systems. *Computer Physics Communications*, *184*(4), 1234–1240. https://doi.org/10.1016/j.cpc.2012.11.019

Keaveney, J., Adams, C. S., & Hughes, I. G. (2018). ElecSus: Extension to arbitrary geometry magneto-optics. *Computer Physics Communications*, *224*, 311–324. https://doi.org/10.1016/j.cpc.2017.12.001

Manzano, D. (2020). A short introduction to the Lindblad master equation. *AIP Advances*, *10*(2), 025106. https://doi.org/10.1063/1.5115323

Miller, B. N., Meyer, D. H., Virtanen, T., O'Brien, C. M., & Cox, K. C. (2024). RydIQule: A graph-based paradigm for modeling Rydberg and atomic sensors. *Computer Physics Communications*, *294*, 108952. https://doi.org/10.1016/j.cpc.2023.108952

Nagib, O., & Walker, T. G. (2025). *Exact steady state of perturbed open quantum systems* (No. arXiv:2501.06134). arXiv. https://doi.org/10.48550/arXiv.2501.06134

Renaud, J. P. (2022). CyRK - ODE integrator implemented in cython and numba. In *GitHub repository*. GitHub. https://doi.org/10.5281/zenodo.7093266

Richardson, D., Dee, J., Kayim, B., Sawyer, B., Wyllie, R., Lee, R., & Westafer, R. (2023). *Study of Angle of Arrival Estimation with Linear Arrays of Simulated Rydberg Atom Receivers*. TechRxiv. https://doi.org/10.36227/techrxiv.24236953.v1

Robertson, E. J., Šibalić, N., Potvliege, R. M., & Jones, M. P. A. (2021). ARC 3.0: An expanded Python toolbox for atomic physics calculations. *Computer Physics Communications*, *261*, 107814. https://doi.org/10.1016/j.cpc.2020.107814

Rochester, S. (2008). *AtomicDensityMatrix*. Rochester Scientific. https://www.rochesterscientific.com/ADM/

Santamaria-Botello, G., Verploegh, S., Bottomley, E., & Popovic, Z. (2022). *Comparison of Noise Temperature of Rydberg-Atom and Electronic Microwave Receivers* (No. arXiv:2209.00908). arXiv. https://doi.org/10.48550/arXiv.2209.00908

Šibalić, N., Pritchard, J. D., Adams, C. S., & Weatherill, K. J. (2017). ARC: An open-source library for calculating properties of alkali Rydberg atoms. *Computer Physics Communications*, *220*, 319–331. https://doi.org/10.1016/j.cpc.2017.06.015

Su, K., Behary, R., Aubin, S., Mikhailov, E., & Novikova, I. (2024). *Two-photon Rydberg*

EIT resonances in non-collinear beam configurations (No. 18035). opticaopen. https://doi.org/10.1364/opticaopen.27941730.v1

Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., ... van Mulbregt, P. (2020). SciPy 1.0: Fundamental algorithms for scientific computing in Python. *Nature Methods*, *17*(3), 261–272. https://doi.org/10.1038/s41592-019-0686-2