

# PYTOMIC: A PYTHON TOOL FOR POLARIZED ATOMIC BEAM TRACKING\*

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## Abstract

Pytomic is a new tool for the simulation and analysis of atomic beams through magnetic systems. It is written in Python and based on the same fundamentals as other particle tracking codes but for atomic beams instead of charged beams. In this case, the manipulation and control of neutral atomic beams is via a force due to the spin interacting with a magnetic field gradient. An object-oriented tool was developed to aid in the design of a beamline through the manipulation of modular elements. The Python language allowed for a smooth implementation and kept the code clear and simple. The primary purpose of developing this code was to have a tool to design, simulate, and optimize a Breit-Rabi Polarimeter to measure the polarization of an atomic beam. In this case, different set-ups with different magnets need to be simulated and optimized for direct comparison. In addition to simulation and tracking modules, a new data analysis module was developed to be able to quickly analyze simulation results, gaining insight from each iteration of the simulation, leading to an efficient and rapid design process. Example applications to design polarimeters for atomic beams with different requirements will be presented.

## INTRODUCTION

Argonne National Laboratory (ANL) was one of the pioneering labs in the development of laser driven polarized targets and sources of polarized atomic hydrogen and deuterium [1-3]. This development has led to the polarized target experimental program at HERMES, DESY, Heidelberg, Germany. Taking advantage of the recent developments in this field, ANL started an R&D effort to develop a novel hybrid spin-exchange optical pumping (SEOP) polarization process that can be used to produce polarized ion beams of deuterium, helium, neon, and xenon. This process leverages Jefferson Lab polarized fixed target technology [4] and is complementary to the meta-stability exchange polarization (MEOP) process which is unique to  $^3\text{He}$  and well developed by a MIT-BNL collaboration [5].

The polarized atomic beams can then be injected into an ion source to produce polarized ion beams for the Electron-Ion Collider (EIC). Achieving a high degree of polarization is very important for injection of the atomic beam, therefore, it is critical to understand the sources of depolarization through the atomic beam transport system. To accurately measure these depolarizing effects, a Breit-Rabi polarimeter which consists of a series of permanent-magnet multipoles, collimators, and a quadrupole mass analyzer, is being designed and built.

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In the effort to design and optimize a Breit-Rabi Polarimeter to measure the polarization of an atomic beam, a new tool was developed in Python language. This new tool allows the simulation and analysis of atomic beams through a magnetic system. It is based on the same fundamentals as other particle tracking codes but for atomic beams instead of charged particle beams. In this case, the manipulation and control of neutral atomic beams are via a force due to the spin interacting with a magnetic field gradient. The tool was developed in an object-oriented approach to aid in the design of a beamline through the manipulation of modular elements. The Python language allowed for a smooth implementation and kept the code clear and straightforward. In addition to simulation and tracking modules, a new data analysis module was developed to be able to quickly analyze simulation results, gaining insight from each iteration of the simulation, leading to an efficient and rapid design process.

## PYTOMIC CODE

### Fundamentals

The forces,  $F$ , exerted by a  $2n$ -pole magnet with an inhomogeneous field,  $B$ , on a particle with a magnetic moment,  $\mu$ , is directed along the radius,  $r$ , and is given by [6]:

$$F_{2n} = -\nabla U = -\frac{\partial U}{\partial B} \nabla B_{2n} = -\mu \frac{\partial B_{2n}}{\partial r} \frac{r}{r} \quad (1)$$

$$F_{2n} = -\mu \frac{(n-1)B_{max}}{(r_{max})^{n-1}} r^{n-2} e_r. \quad (2)$$

If  $\mu > 0$ , this force is radial pointing towards the magnet axis (focusing) and from the magnet axis (defocusing) if  $\mu < 0$ . Vector  $e_r$  is directed towards increasing gradient  $\nabla B_{2k}$ .

- Quadrupole,  $n = 2$ :

$$F_4 = -\mu \frac{B_{max}}{(r_{max})} e_r \quad (3)$$

- Sextupole,  $n = 3$ :

$$F_6 = -\mu \frac{2B_{max}}{(r_{max})^2} r = -\mu \frac{B_{max}}{(r_{max})} \frac{2r}{r_{max}} e_r. \quad (4)$$

Due to their radial dependence of focusing fields, sextupole magnets are most commonly used.

From Eq. (2) and fixing the integration step in the longitudinal direction, all the coordinates can be calculated through any magnet from the kinematic equations. On the other hand, because the approximation of short magnets is

common, an alternative way is often used to track and check the particles focusing. This way is based on the fact that the refraction experienced by a particle through a short magnet can be approximated by a path on a circular arc with the centripetal force [7]

$$f = \frac{mv^2 r_{pt}^2}{2 \mu_B B_{pt} l}. \quad (5)$$

### Object-oriented Structure and Implemented Functionalities

The tool was developed in an object-oriented approach to aid in the design of a beamline through the manipulation of modular elements. There are two main hierarchical class structures, one for the definition of the beam and another for the definition of the beamline, see Fig 1.

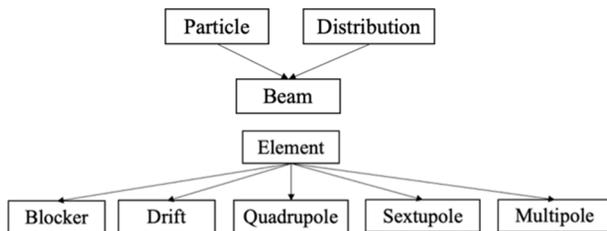


Figure 1: The two main hierarchical class structures in the code: the definition of the beam and the magnetic elements.

The position distribution can also be generated through a tube following a molecular flow tracking. Beamline elements that have been implemented include: sextupoles, quadrupoles, tubes, beam blockers, and a particular element called multipole. This last element allows for overlapping different magnetic fields with offsets to create different non-uniformities and possible errors at random places at the level of a given uncertainty. The elements can also be placed with offsets allowing different set-ups for simulation.

The rates given below are calculated to help optimize the polarimeter design:

$$\text{Loss rate} = \frac{\# \text{ particles with spin} > 0 \text{ at the detector}}{\text{total} \# \text{ particles with spin} > 0} \quad (6)$$

$$\text{Contamination} = \frac{\# \text{ particles with spin} < 0 \text{ at the detector}}{\text{total} \# \text{ particles at the detector}} \quad (7)$$

### Code Benchmarking

One crucial step for every new simulation tool is to benchmark it against other simulation tools or experimental results. Following the comparison and good agreement of the code's results with analytical tracking approximations, the goal is to reproduce the results from different experimental set-ups [6-8]. For example, Fig. 2 shows the velocity distribution of a hydrogen molecular beam at the detector with the same set-up as in [6], and which reproduces the results therein. Notice that comparing with

PyTomic, an approximated error of 0.002 rad in the focusing was found. It might be due to small differences in the precision of the parameters' values.

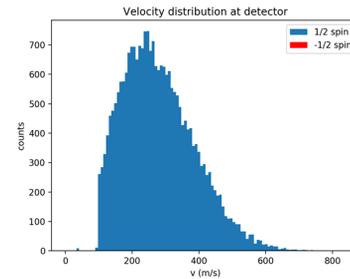


Figure 2: Velocity distribution at the detector for a hydrogen molecular beam following the same set-up and conditions as in [6]. Blue refers to particles with positive spin moment projection and red would be for negative momentum if there were at the detector.

## SIMULATIONS AND RESULTS

Following the successful benchmarking of the code, it was used to simulate and optimize different polarimeter setups using different beams such as hydrogen, deuterium and later 21-neon in order to design and build the appropriate polarimeter. See Table 1 for the parameters of each beam used in the following simulations.

Table 1: Parameters for the Beams Used in the Simulations

Atom	Mass	$\mu$	$\mu \sim \text{due to}$	Spin
Hydrogen	$\sim 1.67e-27$	$\sim 1.86e-23$	Electron	1/2
Deuterium	$\sim 3.34e-27$	$\sim 1.86e-23$	Electron	1/2
21-Neon	$\sim 3.49e-26$	$\sim 3.34e-27$	Nuclear	3/2

Notice that for a neon beam the polarization comes from the atomic nucleus, unlike hydrogen and deuterium where it comes from the electrons. Therefore, the magnetic moment is three to four orders of magnetic weaker, which makes the magnetic selection and detection of the different spin states significantly more challenging.

Different set-ups with different magnets were simulated and optimized for direct comparison. Two main setups were studied: a tube with an offset and a tube with a coaxial inner tube blocking the beam from being close to the axis where the force is weaker. After the initial tube, conditioning the particle distribution, the sequence for the beamline follows: element-drift-element-drift where element can be a quadrupole, a sextupole, or a multipole.

### Hydrogen and Deuteron Polarimeter

A magnet system of short sextupole magnets with high pole-tip fields optimized for hydrogen shows the same behavior for deuterium because the focal length, Eq. (5), is the same for thermalized hydrogen and deuterium atoms [7].

Therefore, based on the first studies for hydrogen atoms, the specifications for the sextupole magnets were determined, which are permanent-magnet Hallbach arrays [9] of 1 Tesla, 25 mm aperture and 10 cm long.

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Figure 3 shows the polarimeter setup optimized for both hydrogen and deuterium beams. It consists of two sextupoles, a beam blocker (20 mm aperture) and a quadrupole mass analyzer (31.75 mm aperture). This design maximizes the transmission of the atoms with the desired polarization while minimizing the contamination from other spin states. Figure 4 shows the simulation results for hydrogen and deuterium atomic beams extracted at the oven operating temperature of 200 °C. It's worth noting that at the same temperature, hydrogen and deuterium are affected the same way by the magnetic field, as explained above.

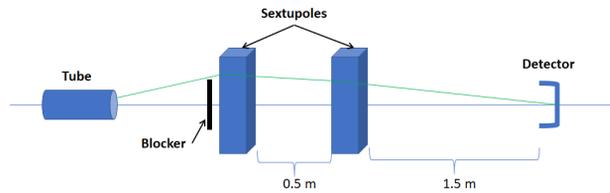


Figure 3: A Breit-Rabbi polarimeter setup optimized for atomic beams of hydrogen and deuterium. The green trace shows the trajectory of an atom focused into the detector by the magnetic field of the sextupoles.

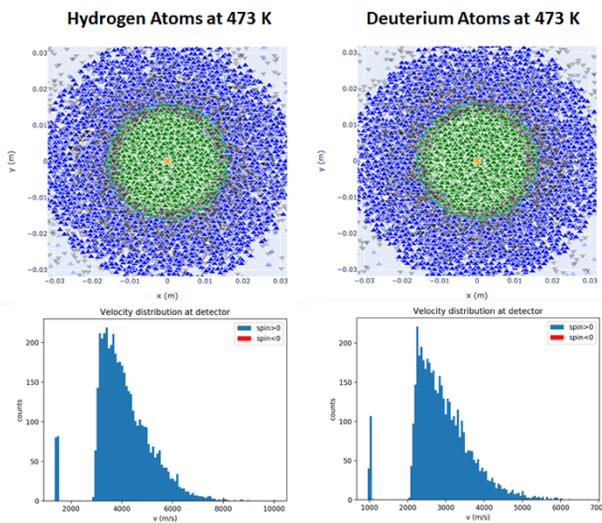


Figure 4: Results of tracking simulations for both hydrogen (left) and deuterium (right) at 200 °C from the source end-tube to the detector. Shown in the top are particle coordinates at the detector plane. The green dots are atoms of interest accepted in the detector while in blue are lost atoms, in black are atoms of opposite spin being rejected. The bottom plots are the velocity distributions of the selected atoms accepted in the detector.

### Neon Polarimeter

After the hydrogen/deuteron polarimeter design, simulations with 21-neon beam were carried out using the same magnetic system. Figure 5 shows a preliminary layout of the polarimeter re-arranged for the selection and detection of neon spin states.

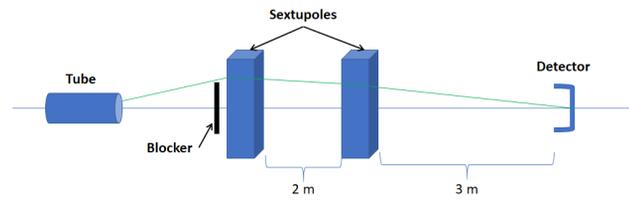


Figure 5: A preliminary Breit-Rabbi polarimeter setup for the selection and detection of a polarized neon atomic beam.

This setup with 21-neon extracted at the oven operating temperature of 200 °C gives a high contamination rate, up to 50%, because the polarization comes from the atomic nucleus. In addition, the loss rate is ~ 60%. To be able to remove any contamination, the detector's aperture must be reduced or the distances between magnets and to the detector increased. See Fig. 6 for the results of a 21-neon beam with different detector apertures. Where the contamination is reduced by using a smaller aperture at the expense of increased particle loss.

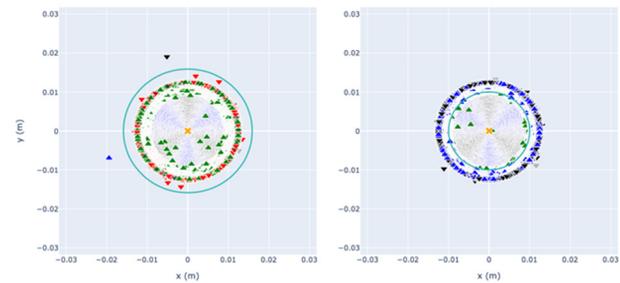


Figure 6: Particles coordinates at the detector plane. The green dots are atoms of interest accepted in the detector while in blue are the lost ones. On the other hand, in red are atoms of opposite spin being accepted in the detector, while in black are the lost ones. (Left) Detector with 31.75 mm aperture. (Right) Detector with 20 mm aperture and no contamination (no atoms in red).

## CONCLUSIONS AND FUTURE WORK

Significant progress has been made in the modelling and design optimization of the Breit-Rabbi polarimeter by using Pytomic. Pytomic is a tracking code for atomic beams that serves for the simulation and optimization of Breit-Rabbi polarimeters. It has been used so far for the simulation and design of a Breit-Rabbi polarimeter for both hydrogen/deuteron and 21-neon atomic beams given the sextupoles' dimensions and field. The polarimeter design is flexible and can be re-arranged depending on the polarized atomic beam under study. In the future, it would be useful to add the radio frequency transitions to be able to select the different spin states one at a time in order to determine the polarization composition of the whole beam, allowing a complete polarimeter simulation.

## REFERENCES

- [1] K. P. Coulter *et al.*, “An active storage cell for a polarized gas internal target”, *Nucl. Instrum. Methods Phys. Res., Sect. A*, vol. 350, pp. 423–429, 1994.  
doi:10.1016/0168-9002(94)91243-2
- [2] R. J. Holt, “Polarized Gas Targets for Storage Rings”, *J. Phys. Colloques*, vol. 51, pp. 205-220, 1990. doi:10.1051/jphyscol:1990617
- [3] M. Poelker *et al.*, “Laser-driven source of spin-polarized atomic hydrogen and deuterium”, *Nucl. Instrum. Methods Phys. Res., Sect. A*, vol. 364, pp. 58–69, 1995. doi:10.1016/0168-9002(95)00281-2
- [4] M. V. Romalis, “Hybrid Optical Pumping of Optically Dense Alkali-Metal Vapor without Quenching Gas”, *Phys. Rev. Lett.*, vol. 105, 2010. doi:10.1103/physrevlett.105.243001
- [5] J. Maxwell *et al.*, “Development of a Polarized Helium-3 Source for RHIC and eRHIC”, *Int. J. Mod. Phys.: Conf. Ser.*, vol. 40, p. 1660102, 2016.  
doi:10.1142/s2010194516601022
- [6] A. V. Yurchenko, D. M. Nikolenko, I. A. Rachek, D. K. Toporkov, and Y. V. Shestakov, “Simulation of Motion of H2 and D2 Molecules in Sextupole Magnets”, *Tech. Phys.*, vol. 64, pp. 1248–1259, 2019.  
doi:10.1134/s1063784219090226
- [7] I. Brunn, “Optimization of the magnet system of the Breit-Rabi polarimeter and calibration of the target gas analyzer of the HERMES experiment at DESY”, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany, Rep. DESY-HERMES-01-74, Apr. 2001.
- [8] Y. V. Shestakov, D. M. Nikolenko, I. A. Rachek, D. K. Toporkov, and A. V. Yurchenko, “Nuclear-Polarized Hydrogen/Deuterium Molecular Source”, *Phys. Part. Nucl.*, vol. 50, pp. 513–519, 2019.  
doi:10.1134/s1063779619050204
- [9] P. Schiemenz, A. Ross, and G. Graw, “Permanent sextupole magnets for polarized Stern–Gerlach-type atomic beam sources”, *Rev. Sci. Instrum.*, vol. 63, pp. 2634–2635, 1992.  
doi:10.1063/1.1142862