Pytomic: A Python Tool for Polarized Atomic Beam Tracking

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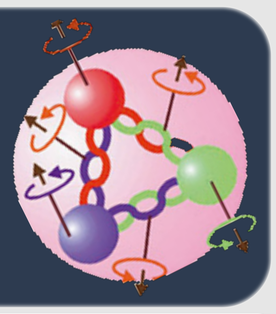


Abstract

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. Therefore, 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.

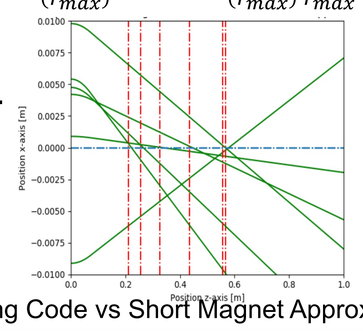
Introduction

Fundamentals

- The forces exerted by the 2n-pole magnet on the particle is directed along the radius and is given by

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

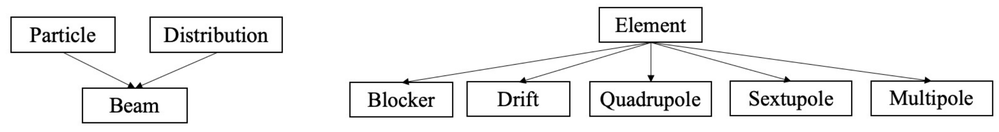
- If $\mu > 0$, this force is directed along the radius towards the magnet axis (focusing) and from the magnet axis (defocusing) if $\mu < 0$. Vector e_r is directed towards increasing gradient ∇B_{2k}.
- **Quadrupole** (n=2): $F_4 = -\mu\frac{B_{max}}{(r_{max})}e_r$ **Sextupole (n=3):** $F_6 = -\mu\frac{2B_{max}}{(r_{max})^2}r = -\mu\frac{B_{max}}{(r_{max})}\frac{2r}{r_{max}}e_r$
- **Loss rate** $\left(=\frac{\#\ particles\ with\ spin>0\ that\ hit\ the\ detector}{total\ \#\ particles\ with\ spin>0}\right)$ and **contamination rate** $\left(=\frac{\#\ particles\ with\ spin<0\ that\ hit\ the\ detector}{total\ \#\ particles\ that\ hit\ the\ detector}\right)$.
- Short magnet approximation: the refraction experimented by a particle through a short magnet can be approximated by a path on a circular arc with the centripetal force: $f = \frac{mv^2 r_{pt}^2}{2\,\mu_B B_{pt}\,l}$



Tracking Code vs Short Magnet Approximation.

Object-Oriented Structure

- The initial atomic beam can be generated with **different distributions** in position, and Maxwell and cosine distributions for the velocity amplitude and direction, respectively. The position distribution can also be generated through a tube following a molecular flow tracking.
- **Hierarchical structure**:

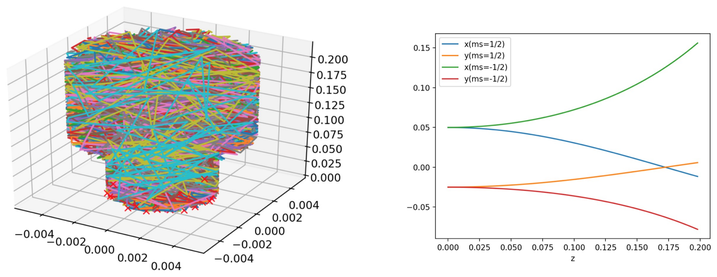


- This last element allows for overlapping different magnetic fields with offsets to create different **non-uniformities** and possible **errors** at random places at the level of a given uncertainty.
- The elements can also be placed with **offsets** allowing different set-ups for simulation.

Simulations and Results

Molecular Flow and Particle Tracking

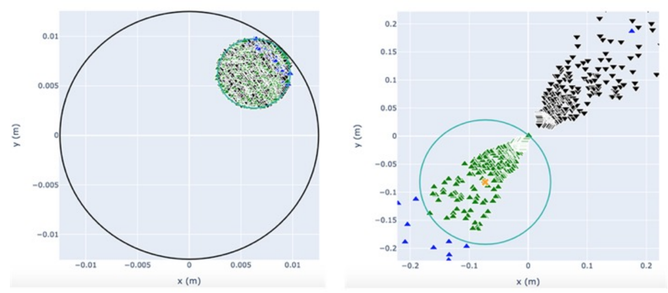
- (Left) **Molecular flow through a tube** with different diameters to generate a distribution of particles for the polarimeter.



- (Right) **Tracking four hydrogen atoms through a sextupole.** The atoms are at two different initial positions and have different spin states

Off-set configuration

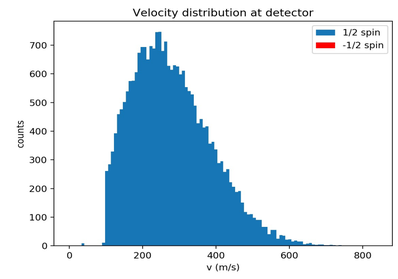
- Setup: **Offset Tube – Sextupole – Sextupole – Detector**.



- (Left) Atomic beam with different polarization components incident on the polarimeter. The beam is offset for better separation by a magnetic sextupole field. (Right) Separation of different polarization components with the possibility of selecting and measuring strength of individual components.

Benchmarking

- Benchmarked it against other simulation tools [1]. Using the same setup than [1], the **velocity distribution at the detector** for the hydrogen molecular beam from Pytomic matches [1].

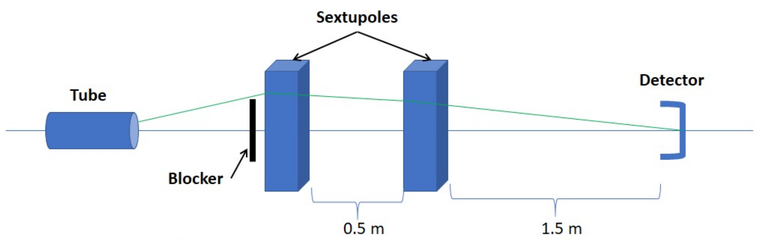


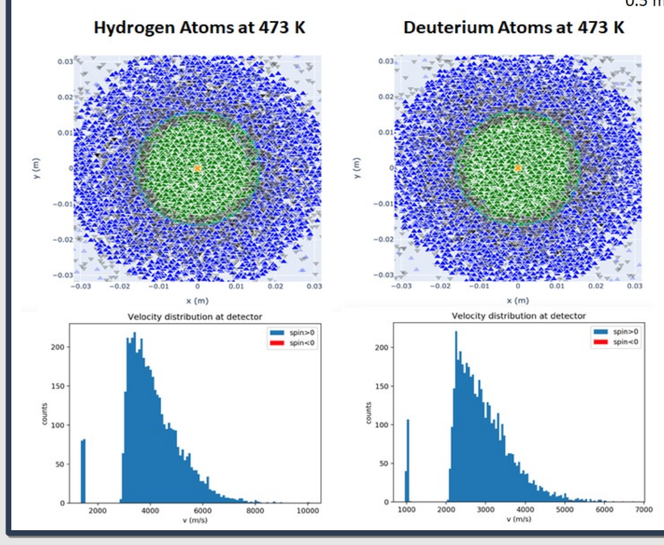
- It was found an approximated error of 0.002 rad in the focusing, that might come from hydrogen molecule parameters used.

Hydrogen and Deuteron Polarimeter

Standard Setup using ⇨ **Blocker** (aperture: 20 mm) - **Sextupoles** (field: 1 T, aperture: 25 mm, length: 100 mm) - **Detector** (aperture: 31.75 mm).

- 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:



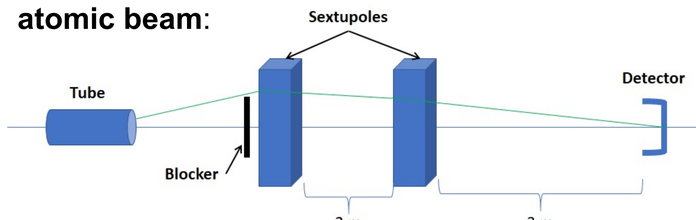


- Results of tracking simulations for both **hydrogen** (left) and **deuterium** (right) at 200 °C from the source end tube to the detector. Shown in the top are particle coordinates at the detector plane. The green dots are **atoms of interest accepted in the detector** while in blue are **lost atoms**,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

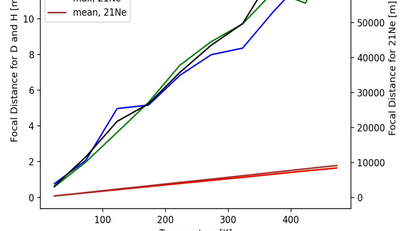
21-Neon Polarimeter

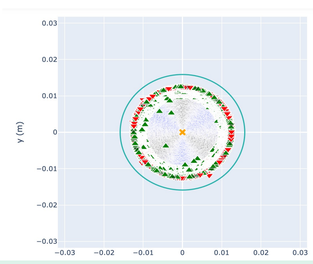
Atom	Mass	μ	$\mu - due\ to$	Spin
Hydrogen	~1.67e-27	~1.86e-23	Electron	1/2
Deuteron	~3.34e-27	~1.86e-23	Electron	1/2
21-Neon	~3.49e-26	~3.34e-27	Nuclear	3/2

- Preliminary Breit-Rabbi polarimeter setup for the selection and detection of a **polarized neon atomic beam**:



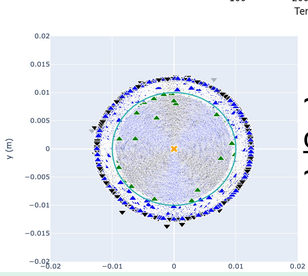
- How the maximum and the mean **focal distance [m]** of a given sextupole vary with the **Temperature [K]** of a beam of hydrogen, deuteron and 21-neon:





~ 50% contamination rate
~ 60% loss rate

Detector with **31.75 mm** aperture



~ 0% contamination rate
~ >99% loss rate

Detector with **20 mm** aperture

Conclusion and Future Steps

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. In the future, it would be useful to add the radio frequency transitions to complete the polarimeter scheme simulation and eventually the nuclear polarization calculations.

References

[1] Yurchenko, A.V., Nikolenko, D.M., Rachek, I.A. *et al.* Simulation of Motion of H_2 and D_2Molecules in Sextupole Magnets. *Tech. Phys.* 64, 1248–1259 (2019). https://doi.org/10.1134/S1063784219090226

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