



DESIGN AND OPTIMIZATION FOR ZEEMAN SLOWER ESPAÑA

USER GUIDE

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Real Instituto y Observatorio de la Armada

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0. SCOPE

The *Real Instituto y Observatorio de la Armada (ROA)* is the institution responsible for the local realization of the Coordinated Universal Time in Spain, UTC(ROA), keeping and maintaining the national time standard, and disseminating the UTC(ROA) time scale where the Spanish's legal time is based on. In our road to the consecution of an optical lattice clock, we have developed this tool that might be of interest to the scientific community.

This tool, which we named *DOZE – Design & Optimization for Zeeman slowers España*, allows to run a series of calculations so as to slow down the atomic beam by using the Zeeman effect with permanent magnets.

The Zeeman effect consists of splitting atoms spectral lines into several components in the presence of a static magnetic field (B). Since lines separation depends on the B field strength, we benefit from the Doppler effect in order to compensate for and keep the atoms in resonance as they move forward towards a counterpropagating laser light field.

As it is not a commercial software, its purpose and functionalities possess certain limitations. DOZE should be used as a guide and aid for Zeeman design and optimization, but final construction and implementation relies on users. ROA disregards any damage or error derived from the usage of this tool.

1. DESIGN CONSIDERATIONS

There are multiple ways of facing the design of a Zeeman slower apparatus and all of them starts with the selection of a suitable atomic transition, a broad-linewidth transition that allows atoms to absorb photons from a laser source. Atoms move in a certain direction and laser beam is counterpropagating. If the transition is in resonance with the laser power atoms absorb a photon from the laser beam and relax spontaneously quickly — depending on the transition linewidth —, being ready for a new absorption. Photons absorbed reduce atom velocity always in the same direction, while spontaneous relaxations accelerate atoms again in random directions. After a lot of cycles, absorption has reduced atom speed while emission mean contribution is around zero:

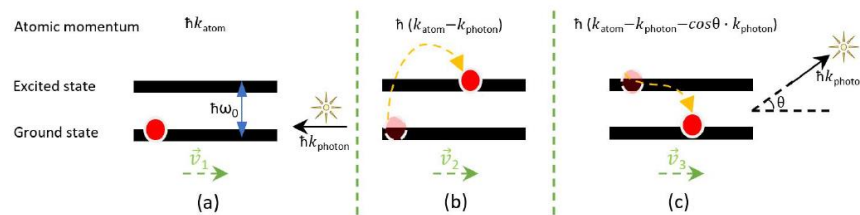


Figure11: (a) Laser cooling of a two-level atom interacting with a resonant laser field in terms of linear momentum exchange. The absorption process (b) reduces the linear momentum of the atom and (c) the spontaneous emission produces an additional, random variation of its momentum, which is reduced to zero when integrated for many interactions.

As atoms slow down, they perceive a different frequency from the laser due to the Doppler effect and resonance is lost unless this effect is compensated for. By means of a magnetic field, the transition energy, i. e., its frequency transition, is modified as needed. If carefully designed, Doppler effect can be compensated and atoms are kept in resonance —and available for photon absorption— within a certain distance. It must be noted

that there is a minimum distance constraint: as each absorbed photon removes $\hbar k$ kinetic momentum from atoms, slowing atoms from a high velocity to a much lower one requires a certain number of photon absorption and each of them takes a mean time inversely proportional to the transition linewidth (see [Table 2.1](#), at the end of [Atomic kinetics](#) section).

DESIGN FLOW

To create a Zeeman slower apparatus, the design flow to be done with DOZE runs like this:

- Choice of the atoms class of velocities to be slowed down and the final target velocity they should have.
- Selection of the distance for the deceleration.
- Derivation of the deceleration needed to achieve the goal.
 - Deceleration a achieved depends on the radiation pressure force which formula includes laser power ($s=I/I_{sat}$), real detuning perceived by atoms Δ , the transition linewidth γ , atoms mass m and wavenumber k . For a certain atomic species –sets linewidth and mass–, deceleration will only depend on the laser power and the detuning.
- Calculation of the Doppler effect they will perceive on the laser source is performed.
- Derivation of the Zeeman effect needed is the one that compensates the Doppler effect by the design of a transversal magnetic field along the deceleration zone, trying to make $\Delta(z,v)=0$

$$\Delta(z, v) = \Delta_0 + kv(z) - \mu_{\text{eff}} B(z)/\hbar.$$

- Position of the cylindrical magnets (quantity, size and remanence user determined) can automatically be located to achieve the needed magnetic field.
- Accomplished previous step, a simulation on the atomic kinetics can be performed: atoms at some different velocities are entering the deceleration zone and atom behaviour is analysed:
 - First, magnetic field is calculated at the position where atoms are. Its value will depend on the magnets position, shape and remanence.
 - A calculation of atoms perceived detuning is made. This calculation indicates if they are in resonance with the laser source.
 - Then, the deceleration they perceive by the influence of the laser field and the detuning calculated previously.
 - Considering acceleration is constant along a differential time step ($1 \mu\text{s}$ or less is resolution good enough), new velocities are calculated and the loop starts again until all time steps are computed.

RESTRICTIONS PRESENT IN DOZE

Some design factors on the way DOZE works do not appear on the GUI but can be loaded from a [config.ini](#) file to be brought into the calculations.

Note that there are also some ideas relying under the way DOZE works that cannot be modified and that are important to understand the way it is thought and for its proper use:

- **Magnets are cylinder shaped.** Their size and magnetic power can be modified but the shape is fixed and cannot be changed unless the source code is modified.
- **Magnetic field is transverse** to the atoms and laser beam axis. Longitudinal B field has been not considered in the DOZE tool.



Figure 1.2.
Cylindrical magnet

- Ideal magnetic field is calculated strictly to get the atoms from the defined capture velocity to the final velocity within a distance called "Deceleration length"; the **ideal B field** is supposed to be zero outside this zone, causing an **important discontinuity**. As the field generated by magnets can never reproduce this B field, two additional pairs of magnets are located outside the deceleration length causing the apparatus to be somewhat longer. The first pair of magnets is used to control the slope entry of the B field at the beginning of the deceleration zone while the last pair is used to control the B field extinction beyond the deceleration zone and for final speed fine adjustment. For these reasons:
 - **Certain B field exists outside the deceleration zone.** This usually leads to capture atoms a bit quicker than decided and to slow them down a bit more than the value set in the tool. That is why atomic kinetics function is needed: to really analyse if desired deceleration of the atoms is met. If not, user can play around with the parameters to achieve it. To handle this a scaling parameter is introduced in the tool, and explained in the following paragraph.
- To avoid excessive deceleration, the **required B field profile is deliberately divided by a factor** (by default $k=1.05$). If it were $k=1.0$, the B field existing outside deceleration zone would slow down the atoms more than required and they will probably turn back to the oven. Lowering a bit by this $k=1.05$ factor will compensate the excessive slowing due to residual existing B field outside deceleration length. This factor can be modified in [config.ini](#) file under section `[scale_factor_B]`.
- The **automatic optimization process explores magnet positions in the y-direction** (approximating or separating magnets from the tube axis) but not in the z-direction. Nevertheless, the user can move magnets with the spinboxes within the lower left side of GUI and move them in the z-axis. After that, running optimization process will respect the z-positions the user chose.
- In the optimization process, **first and last pair of magnets are moved integrally with the pairs next to them ("partners")**. Both are closer to the tube than their partners and the value in [mm] can be adjusted in [config.ini](#) file. Nevertheless, those first and last pair of magnets can be moved afterwards manually using their corresponding spinboxes and run the atomic kinetics again.
- In atomic kinetics simulation, **atoms move ONLY along the z-axis**. The purpose behind this DOZE tool is to assist the user with the apparatus design but not to analyse its efficiency. This is, beam alignment, oven atomic flux collimation, etc. is out of the scope of the DOZE tool.
- **Transition is considered as an ideal closed two level.** This means that atoms are excited to a single electronic state and relaxed back to the initial one; there is no atom loss due to third states either to ground or excited split states that may lead to dark states.
- **Magnetic field must cross $B=0$ line at some point**, leaving at least two pairs of magnets on each side. DOZE will raise a warning if this does not happen and will recommend modification of laser detuning and/or velocities.
- **Laser power is assumed to have the polarization needed to induce the transition.** Furthermore, by means of [config.ini](#) file, it is possible to consider both circular polarizations, where σ^+ and σ^- exist in the same amount of power (in *Power of Laser [mW]* box). Using both polarizations will show a bit more deceleration: when the B field is outside the deceleration zone, at some points it will show the same values as in the deceleration zone with opposite slope, conducting resonance with the opposite polarization. If the B field is designed for a σ^- circular polarization for $\Delta m = -1$, it will contribute when the B field slope is growing (if μ_{eff} is negative), but at some points the same B field values with opposite slope will momentarily be tuned to σ^+ transition $\Delta m = +1$. When using both polarizations, they will be considered as ideal two-level closed transitions and both will contribute to the atoms slowing: their effects of both of them will be added up.

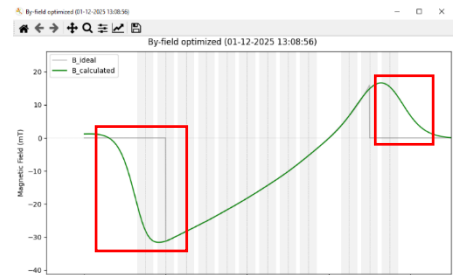


Figure 1.3. Excessive B field outside deceleration zone

2. GUI DESCRIPTION

Graphical User Interface (GUI) is split up to three main blocks:

- Upper left-hand side block contains **input parameters** and values given to the tool for proper calculations.
- Right-hand side block contains a **couple of graphs** where magnets position and field strength are shown where x-axis represents the length of the Zeeman apparatus. At the very opening, these graphs will show the ROA and DOZE logos, but just until input parameters are loaded to the system.
- Middle left-hand side block is the **Buttons area** where some actions or further calculations can be performed.
- Once input parameters are loaded to the system, the lower left side of the GUI will be filled with a **list of spinboxes** which represent magnets position (first column z-position, second column y-position) to adjust their values to see how magnetic field strength changes. This spinboxes can be moved by their containing arrow buttons up-down or also with the arrow-keys on the keyboard and they move units depending on the position of the text cursor.

The GUI is responsive by increasing size of the graphics area -left side part will be kept invariable in size- and has a minimum size of 1280 x 820 px. It is designed for full HD screens 1920 x 1080 px; depending on the screen physical size, windows may adapt font size to pixel size. If user finds problems with fonts partially hidden, in the .exe file right click and select *Properties* -> *Tab Compatibility*, under section *Configuration*, press *Change PPP configuration* and select *Disable behaviour of high PPP by System*.

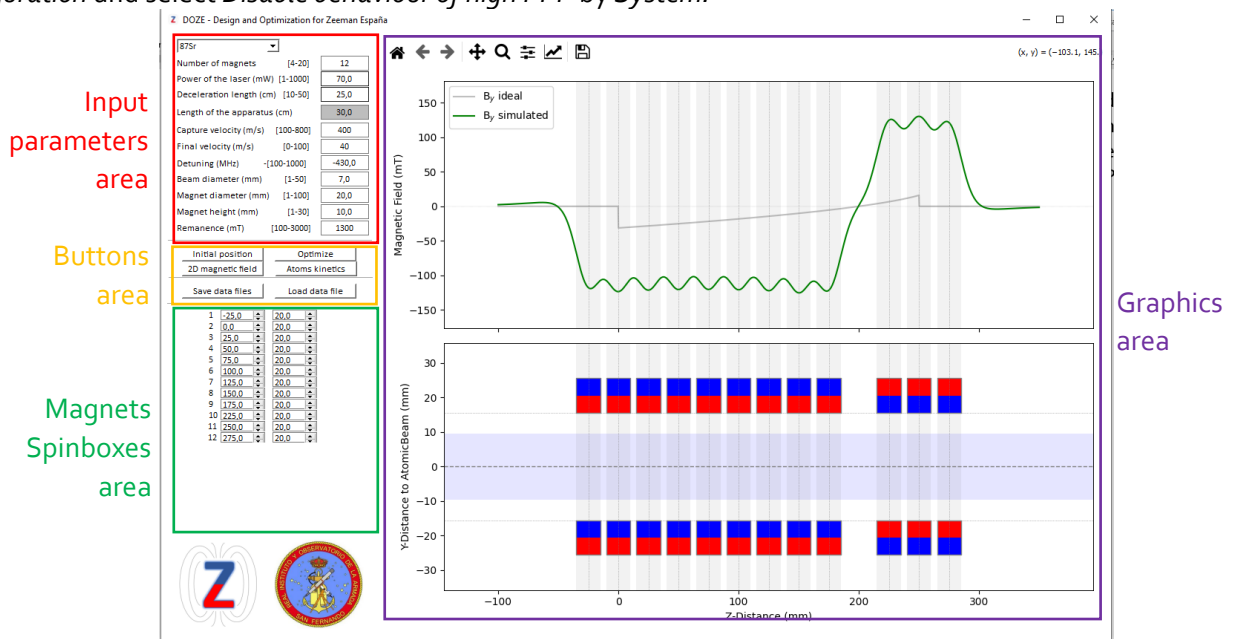


Figure 2.1. GUI main areas.

To show up DOZE's GUI, user can download the tool from this GitHub repository:

<https://github.com/icortes-roa/DOZE---Design-and-Optimization-for-Zeeman-slowers-España>

Both python source code and a binary .exe release are available with the proper instructions.

INITIAL VARIABLES

DOZE would run a usual step-by-step process that starts by setting the initial parameters. In the upper left side of the GUI, the **Input parameters** area will be already filled up with values set in the [config.ini](#) file. There, all parameters **can be changed** (except the length of the apparatus, which is calculated automatically):

- **Combobox/dropdown menu** where to select **atomic species**: strontium (^{87}Sr) or ytterbium (^{171}Yb).
- **Number of magnets** to be used for the Zeeman slower construction. Minimum four pair of magnets (B field has to cross zero leaving two pair of magnets at each side), maximum 20 (spinboxes zone full).
- **Power of the laser** [mW]. Amount of effective CW laser power (assumes the polarization is the one needed to induce the transition selected). Minimum 1 mW, maximum 1000 mW.
- **Deceleration length** [cm]. It is **important to remark** this will be the deceleration line but two additional magnets will be added to control the initial and final slope of the **B** field; so, the real length of the apparatus will be somewhat higher (next parameter Length of the apparatus), depending on the number of magnets selected. Minimum 10 cm, maximum 50 cm.
 - **Length of the apparatus** [cm]. This include the total length from the centre of the first pair of magnets to the centre of the last pairs. It is automatically calculated and cannot be manually modified.
- **Capture and final velocities** [m/s]¹. This will set the maximum entry and final velocities with which the atoms inside the Zeeman slower are supposed to be decelerated. These parameters will define the difference in B field intensity at both sides of the deceleration zone (control the slope of the field).
- **Detuning** [negative MHz]. This parameter indicates how much the laser frequency is red-detuned to match the cooling transition along the Zeeman apparatus. A higher value in absolute value will displace the needed B field upwards. Minimum -100 MHz, maximum -1000 MHz.
 - **IMPORTANT**. Frequency detuning must be chosen in a way that leaves at least two pair of magnets at each side of zero crossing to run properly. Code will prevent it by a pop-up window warning.
- **Beam diameter** [mm]. Diameter of collimated laser beam. Minimum 1 mm, maximum 100.
- **Magnets diameter and height** [mm]. Size of cylinder magnets. Following typical values at neodymium magnets available in common websites, minimum diameter is set to 1 mm while maximum is 100 mm. About height, minimum magnet height is set to 1 mm while maximum is set to 30 mm.
- **Magnetization** [mT]. Remanence of the magnet as described in its datasheet. Indicates the ability of the material to retain the magnetism induced on it. Minimum value is 100 mT, maximum 3000 mT.

LOADING PARAMETERS IN THE SYSTEM

After having all parameters filled up, next step would be loading the parameters into the simulation by pressing button **Initial position**. This will proceed with a first calculation of the needed B field to achieve the desired deceleration and will show an initial distribution of the magnets close to the tube:

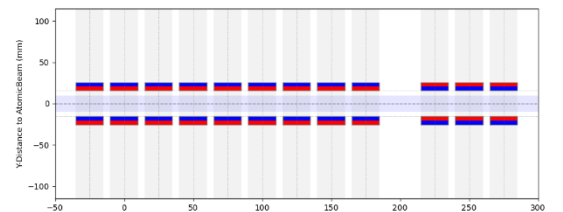


Figure 2.2. Initial distribution of magnets at minimum y-distance

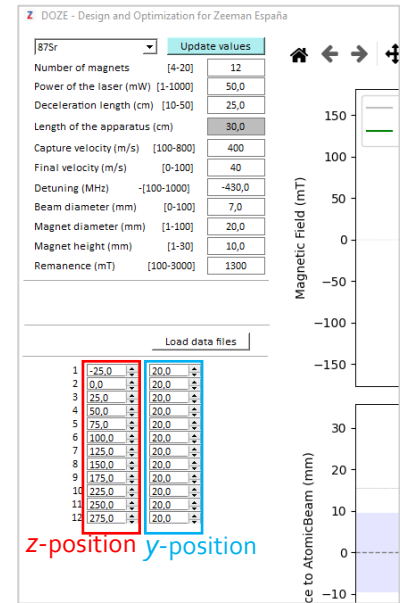
¹ As the real B field generated by the magnets will never match perfectly the ideal B field needed, there will exist a certain B field outside the deceleration zone. Therefore, there will be a difference between both of them that will lead to different values for real capture and final velocities of the atoms previously selected. When the tool optimises automatically the magnets positions, the real capture velocity will usually be a bit greater than settled in DOZE and real final velocity will differ from the target. Simulation made in *Atoms kinetics* button will show better approximation of what would be found in real experiment. This is compensated a bit by using a $k = 1.05$ factor when calculating the ideal B field profile. This factor can be modified in the [config.ini](#) file under section *[scale_factor_B]*.

If any of the **Input parameters** is changed **Initial position** button will disappear and the **Update values** cyan button will appear next to atom combobox. After changing all desired parameters, this **Update values** button has to be pressed and the **Initial position** will be shown up again to load the new values on the system.

After the previous step, a **set of spinboxes** will be shown in the lower left-hand side of the GUI. Each of them represents the position of the magnets (first column represents z-position while second represents y-position). Trying them out by changing values up and down will show how magnetic field created by magnets -**green curve, current B-** changes by, what is especially useful comparing it with the needed field (ideal) to achieve atoms deceleration -**grey line, ideal B-**.

Magnets position can be changed with the spinboxes, but with constraints:

- In the z-axis:
 - They have a range of [-500, 500] mm.
 - They cannot invade the next magnet: minimum distance between magnet centres = magnet diameter.
- In the y-axis:
 - They have a range of [-150, 150] mm.
 - They cannot approach to the tube closer than indicated by **tube radius** + **safety distance**, values that can be changed in [config.ini](#) file.



↑ Figure 2.3. Update values button and spinboxes.

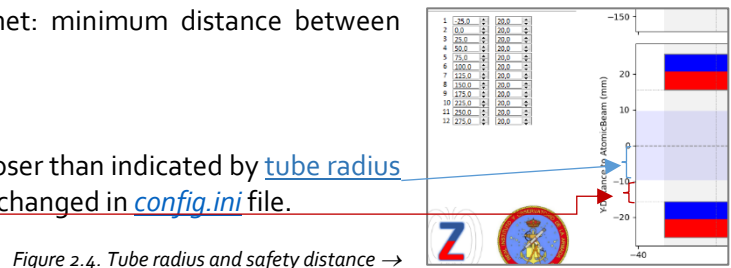


Figure 2.4. Tube radius and safety distance →

Adjusting magnets positions will recalculate in real time the B field generated by magnets, so the user can move them to have the desired magnetic field. Furthermore, in order to find and reach the proper distance for the magnets, there is an automatic process implemented, which is described in next section.

OPTIMIZATION PROCESS

The button **Optimize** will run an algorithm to automatically move the magnets to adapt the B field created by them to the needed B field for atoms deceleration. In this process, all magnets are moving back and forth vertically to adapt the **green curve -the current B-** to the **grey line -the ideal B-** along the deceleration zone. The exceptions are the first and last magnets, whose position is always fixed in relation to their attached magnets (first and last within the deceleration area); this relative position can be modified in the [config.ini](#) file under section [\[data_initial\]](#), block "OTHER PARAMETERS not modifiable in GUI":

- These values will write on variables *self.sep_ini* and *self.sep_last* in script *ZeemanCore.py* in folder *zeeman_package*. These parameters show in mm the distance kept between the initial or final two pairs of magnets. Positive sign indicates initial/last magnet is closer to the atomic beam.

The optimization process runs following this sequence, starting with the initial position:

- Difference between the current B field and the ideal B field within deceleration zone is calculated.
- A magnet is moved a certain distance and the new current B field is calculated:
 - If deviation between the new current and the ideal one is better (lower), it jumps to next magnet.

- If not, it is moved in the other direction and it is rechecked.
- If there are no improvements, the pair of magnets remain at their last position and the next pair starts with the optimization process.
- This process is run until no better deviation can be achieved.
- The process starts again up to five times by moving magnets a smaller distance at a time.

This optimization process can run differently each time:

- It can start by moving the magnets closer to or farther from the tube.
- It can start from the first magnet or from the last one.
- Distances to move them at each round are defined from a parameter in [config.ini](#) file called *displ* under section [\[data_initial\]](#), block "OTHER PARAMETERS not modifiable in GUI". It represents the minimum distance the magnet can be moved and it is the resolution of the system that will host the magnets. In our case, 0.1 mm is the minimum value imposed by our 3D printer machine. Starting with this parameter:
 - First optimization runs at 50 times the value of that parameter *displ* (in our case 5 mm).
 - Second optimization runs at 20 times the value of that parameter *displ* (in our case 2 mm).
 - Third optimization runs at 10 times the value of that parameter *displ* (in our case 1 mm).
 - Fourth and fifth optimizations runs at the value of that parameter *displ* (in our case 0.1 mm), but fourth goes from the last magnet to the first one and fifth the opposite.

Before or after the optimization process, the user can again play around with the **spinboxes to move the magnets** to a desired position and, hence, make whichever adjustments to the B field generated by magnets.

While the optimization process is running, a progress bar will tell the user in which of the five optimization rounds the process is in (20% each) and a **Stop Calculation** button is available.

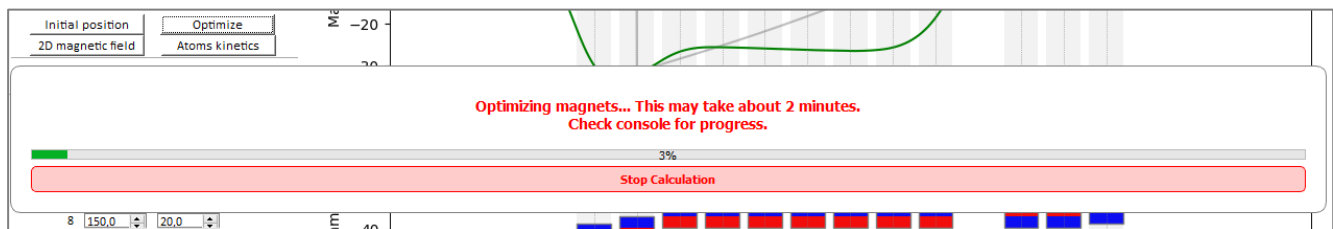


Figure 2.5. Progress bar while optimization process is running. Stop Calculation button allows the user to stop it, leaving magnets in their current position.

By clicking it, the optimization process will stop leaving magnets just where they were at that point. The user can now move magnets again and, if **Optimize** button is pressed, the process will start over the five optimization rounds but taking current magnets positions as initial ones.

Atomic kinetics simulation can be run even when optimization process is not ended as, in reality, the user can simulate whichever B field is desired independently whether or not it slows the atoms down. Precisely, this function is intended to evaluate how well the real B field performs.

2D MAGNETIC FIELD LINES GENERATION

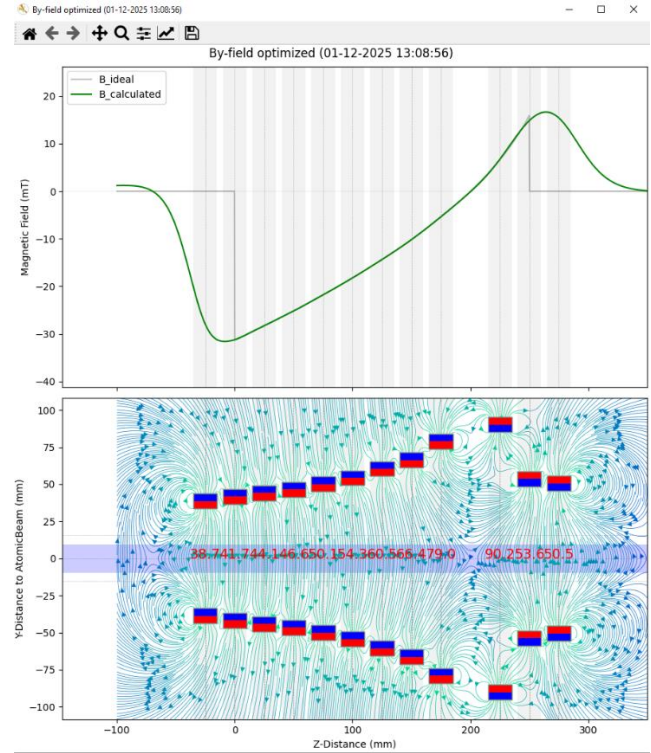
The button **2D magnetic field** will splash a pop-up window with a graphics showing the 2D B field lines created by the magnets with distance from magnets centres to atomic axis.

Basically, it would be an extended view of what is shown in the main screen graphics at current time. This picture can help to search for unexpected behaviour of the magnetic field and provide a clue on how to move the magnets to achieve the desired field.

This button can be pressed anytime if magnets exist in the system -shown in the lower graph of main screen-.

These graphics can be automatically saved later b pressing **Save data files** button, which behaviour is explained in a latter section.

Figure 2.6. Graphics shown up by button "2D magnetic field" →



ATOMIC KINETICS SIMULATION

The **Atoms kinetics** button will start a calculation of how atoms at different speeds are slowed in their way across the Zeeman slower apparatus and will show a graphic with the results. The algorithm flows in this sequence:

- One atom per velocity is created starting at the initial position in z-axis. This position -in [mm]- can be defined by in the *atoms_initial_z_position* parameter in [config.ini](#) file, under section [\[atomic_kinetics\]](#).
- The frequency detuning experienced by the atoms is:

$$\Delta(z, v) = \Delta_0 + kv(z) - \mu_{\text{eff}} B(z)/\hbar,$$

where:

- their velocity $v(z)$ determines detuning caused by the Doppler effect $kv(z)$, being k the wavenumber.
- the current $B(z)$ field generated by magnets at atoms positions determines the detuning caused by the Zeeman effect $\mu_{\text{eff}} B(z)/\hbar$, being μ_{eff} the effective magnetic moment and \hbar the reduced Planck constant,
- Together with the detuning of the laser Δ_0 , the whole detuning $\Delta(z, v)$ is known.
- Knowing the detuning -how in resonance atoms are-, the radiation pressure force each atoms experiment and, divided by atom mass, their deceleration:

$$a = -\frac{1}{m} \frac{s}{1 + s + 4\Delta^2/\gamma^2} \frac{\hbar k \gamma}{2},$$

where m is the atom mass, \hbar is the reduced Planck constant, k is the wavenumber, γ is the decay rate, Δ is the detuning and $s = I/I_{\text{sat}}$ is the intensity over transition saturation intensity, a dimensionless laser intensity parameter that determines the strength of the radiation pressure force.

- Assuming the deceleration is constant along a time step dt , the speed at the next time interval is known, as well as the new z-position where atoms are: $v(z+dt) = v(z) + a(z) \cdot dt$

During the calculation time, loop is repeated until time vector is finished and, then, a pop-up graphics will show up with the results:

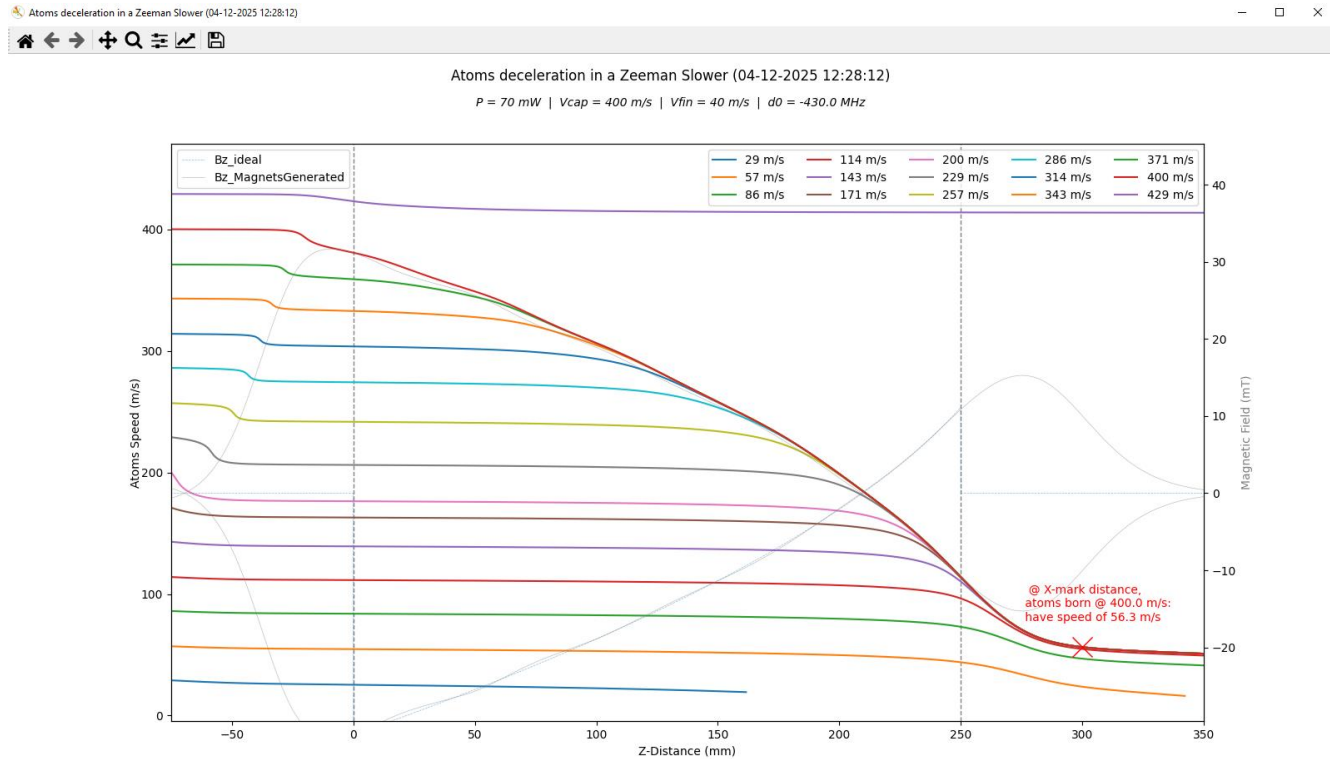


Figure 2.7. Graphics shown up after finishing "Atomic kinetics".

The size and resolution of the time vector can be modified in [config.ini](#) file by changing the corresponding parameters under section [\[atomic kinetics\]](#): resolution of time steps would be dt in [s] while size of vector would be Nt [it is a number #]:

- The longer the vector, the longer the time it will take to the system to compute the atomic kinetics.
- If resolution time is too high, the assumption that acceleration is constant along dt is not valid anymore, and results can show incorrect calculations. On the other hand, if it is too short, user will need a big vector Nt to see how atoms reach the end of the apparatus.

For a standard Zeeman slower of around 30 cm and for capturing speeds of about 500 m/s, $dt=1 \mu s$ and a size of about $Nt = 10.000$ should be enough (total flying time 10 ms).

The amount of different velocities to be simulated can be configured within the [config.ini](#) file under [\[atomic kinetics\]](#) section, parameter N_{vel} . This will create N_{vel} atoms with velocities equally distributed from $V_{cap}/(N_{vel}-1)$ to $V_{cap} + V_{cap}/(N_{vel}-1)$ assuring V_{cap} is one of the velocities to be analysed.

The process will take dozens of seconds to be completed depending on the time vector size, number of velocities to be simulated and the performance of the machine where the code runs.

A progress bar will show the advance of the process that can be cancelled by pressing **Stop calculation** button while it takes place, but cancellation will not show any graphics with results: only 100% finished calculation will show the graphics shown before.

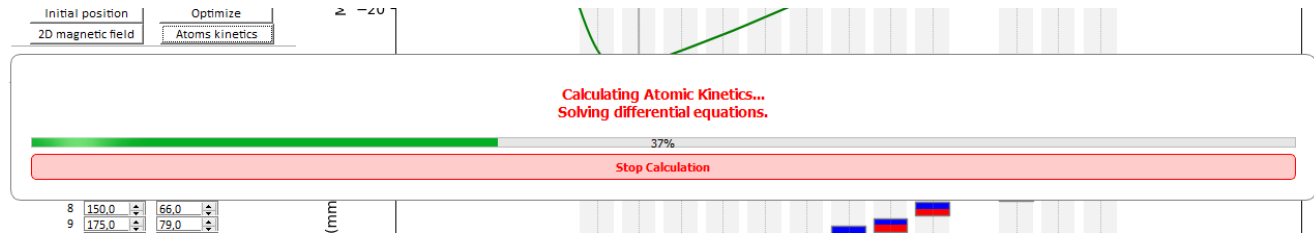


Figure 2.8. Progress bar of "Atoms kinetics" calculation, with **Stop calculation** button.

By default, configuration in [config.ini](#) file, only the direct polarization will be considered (σ^- in case of typical closed transitions with B field positive slope where μ_{eff} is negative²). All power defined in *Power of the laser* parameter will be supposed to be present. If the user wants to check the influence of other polarization σ^+ , parameter *use_sigma_plus* under section [\[data_initial\]](#) can be changed to True and the atomic kinetics will also slow down atoms in zones where B field slope is negative, reducing atoms speed at the end a bit more. Same power is applied to both polarizations.

If, after running atomic kinetics simulation, results are not those expected by users, it would be a matter of changing a bit the parameters given to the system to see how the slower performs:

- Increasing B field at the beginning of the slower will capture faster atoms.
- Moving last couple of magnets will modulate the final atoms speed.

Also, bear in mind that there is a minimum distance to reduce the speed of atoms a certain amount, depending on laser power, capture and final velocities and atoms mass. A table is shown for ^{87}Sr and ^{171}Yb atoms speed reduction, considering maximum acceleration possible is $a_{\text{max}} = -\eta \hbar k \gamma / 2m$ where m is atoms mass, γ is the decay rate, k is the wave number, \hbar is reduced Planck constant and $\eta = s/(1+s)$ where $s = I/I_{\text{sat}}$. In a realistic supposition $\eta = 0.6$ ($I = 1.55 \cdot I_{\text{sat}}$):

Atoms speed reduction desired (m/s)													
	-100	-150	-200	-250	-300	-350	-400	-450	-500	-550	-600	-650	-700
^{87}Sr	8.3	18.7	33.3	52.0	74.9	102.0	133.2	168.5	208.1	251.8	299.6	351.6	407.8
^{171}Yb	15.6	35.2	62.5	97.7	140.7	191.5	250.1	316.6	390.9	472.9	562.8	660.5	766.1
Minimum distance needed to achieve it (mm)													

Table 2.1. Examples of minimum distances needed to reduce some velocities for ^{87}Sr and ^{171}Yb .

Following the table, you cannot expect to slow ^{87}Sr atoms 600 m/s in 30 cm!

² In case μ_{eff} is positive, what is called σ^- along this user manual and the code itself will be in reality σ^+ . Nothing has to be touched within the system, just knowing the names of parameters would be changed.

SAVE DATA FILES

Once some parameters are loaded into the system, which means **Initial position** button has been pressed at least once, **Save data files** button shows up allowing the user to save current data and, if any, generated graphics:

- Pressing the button will create a folder in current working directory, named *YYYYMMDD_SavedData*.
- Inside this folder (with name stating by *HH_MM_SS*) there will be stored:
 - A data file called *simulation_data* in format H5 containing most important parameters loaded in the simulation and some of the vectors created by calculations at the point where user is working. HDF5 file data structure is explained in [chapter 4](#).
 - Last graphics, if any, generated by button **2D magnetic field**, called *Graph_2D_MagneticField*. WARNING: if some parameters are modified but no new 2D magnetic field graphics is generated, DOZE will not create a new graphics to store it; it will take the last one existing in memory (last one generated).
 - Last graphics, if any, generated by button **Atomic kinetics**, called *Graph_Atomic_Kinetics*. WARNING: if some parameters are modified but no new atomic kinetics graphics is generated, DOZE will not create a new graphics to store it; it will take the last one existing in memory (last one generated).

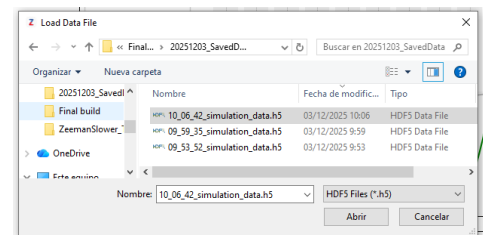
If some parameters are changed in the parameters input area (upper left side of GUI), the **Save data files** button will disappear until buttons **Update values** and then **Initial position** are pressed and this will modify current parameters which can now be saved to file.

LOAD DATA FILE

Once some parameters are loaded into the system, which means **Initial position** button has been pressed at least once, **Load data file** button shows up allowing the user to load data from as pre-existing H5 saved file:

- Pressing the button open a window to navigate to the file to be loaded.
- Once selected, on double click or Open, will load the data into DOZE current set, allowing to recover magnets position and input data

Figure 2.9. Load data browser. →



IMPORTANT NOTE: Data loaded from [config.ini](#) will not be respected, as they will be overwritten in memory by data contained in the H5 file. For instance, if H5 file was saved with *use_sigma_plus = True* but DOZE has been opened with *use_sigma_plus = True*, after loading an H5 this will be overridden and new calculation will be done with *use_sigma_plus = True*.

3. MAIN VARIABLES IN CONFIG.INI FILE

The [config.ini](#) file contains default parameters loaded initially on the GUI and also some variables not usually touched very often in execution time. The user can find their meaning and a short explanation to decide how to adapt them to his/her experiment or simulation.

IMPORTANT NOTE. This [config.ini](#) file is loaded at DOZE start up process. Modification of [config.ini](#) file will not have any influence on the running calculations and processes until DOZE is closed and started up again.

The file start with a short title:

; Sample configuration file

First section involves mainly the default data used for GUI initialization. Most of these parameters can be changed in the GUI itself, but these are the values the user will see when DOZE is fresh started:

[data_initial] [Section title.](#)

<i>Npm=12</i>	Number of pairs of magnets (including the first and last, considered outside the main slowing zone). As a suggestion, number of magnets is related to their size and the distance for the slower. DOZE will warn if there are too many and cannot be arranged, but if the user puts a small Npm or small magnet diameter with big blanks in between, B field profile will have oscillations between magnets and tool will not be able to create a magnetic field similar to the ideal one. Range [4-20].
<i>P=70</i>	Laser power effective for inducing the transition [mW]. The amount of power is supposed to have the right polarization to induce the transition. So, if the user experiment needs circular polarization this P is supposed to have it, meaning the user may need more power for the experiment. Range [1-1000].
<i>z=25</i>	Deceleration length [cm] of the apparatus, not including first and last magnet. This distance represents the zone where designed B field matches as much as possible to ideal B field needed to slow the atoms. Depending on the atoms, the laser power and the deceleration desired, there is a minimum distance needed to achieve it. An indicative table (Table 2.1) is shown in chapter 2 , under section Atomic kinetics simulation . Range [10-50].
<i>V_cap=400</i>	Defined velocity for atoms to be captured. Note that atoms over this speed may be also captured, as real magnetic field does not match exactly the ideal one, existing some extra field before $z=0$. Range [100-800].
<i>V_fin=40</i>	Atoms final velocity at the end of the apparatus. Note that, after atomic kinetics simulation, real atom speed will be different as real magnetic field does not match exactly the ideal one, existing some extra field before after the defined slowing length (over z_{max}). Range [0-100].
<i>do=-430</i>	Laser detuning [MHz]. It is negative as light source is red detuned. Greater absolute value will lead to a needed magnetic field displaced up, like a positive offset to the whole B field curve: initial field smaller (in absolute value), final field greater (in absolute value), zero crossing of the magnetic field moved to left. Range [-100,-1000].
<i>w0=7</i>	Diameter beam waste of the collimated laser beam [mm]. Range [1-50].

<i>mag_diam=20</i>	Magnet diameter (cylindric) [mm]. Range [1-100].
<i>mag_heig=10</i>	Magnet height (cylindric) [mm]. Range [1-30].
<i>Tmagz=1300</i>	Magnet remanence as shown in magnet datasheet [mT]. Range [100-3000].

#----- OTHER PARAMETERS not modifiable in GUI -----, but still in sectin [data_initial]

<i>ext_tube_radius=12</i>	External vacuum tube radius [mm]. Together with the safety margin, it will constrain how close to the atomic beam the magnets can be.
<i>safety_margin=6</i>	Safety distance between magnet and vacuum tube, usually due to free space needed or size of containers and brackets for magnets.
<i>despl=0.1</i>	Resolution of the minimum vertical movement for the magnets [mm] for the optimization of magnets positions. This parameter is related to the resolution in the construction process of the apparatus.
<i>max_iters=30</i>	Maximum number of iterations for each magnet optimization process [#]. Sometimes, depending on the ideal B field, optimization process for magnets position may tend to infinite loops, usually due to zero crossing too close to a magnet: DOZE tries to separate the magnet further and further with minimal influence on generated B field. This way, a top number of iterations is set in the loop. The default value is 30, a value which proved to work well for most of designs tested, but can be changed by user here. A greater number will cause a longer optimization process and better matching generated B field VS ideal B field, while a shorter one will result in a quicker optimization but a worst matching between desired and generated B field.
<i>eta=0.6</i>	Safety margin to be considered for the slowing. Although all power is supposed to be transferred to atoms in a closed transition, the reality is that no transition is completely closed, no magnetic field is perfect and no laser is totally stable in terms of optical power. Parameter <i>eta</i> close to 1 may allow shorter Zeeman slower but more critical in terms of stability, as minimal flaws on magnetic field or laser power will make the slower not to work as expected. Small eta of around 0.4-0.5 will demand long Zeeman slower with problems for vacuum creation and atoms divergence in radial directions. So, values in between 0.6-0.8 are realistic.

Next section includes some values for the atomic kinetics calculations. These parameters can only be changed via the [config.ini](#) file:

[atomic_kinetics] [Section title.](#)

<i>N_vel=15</i>	Amount of different atom velocities to be simulated in atoms kinetics. They will be distributed automatically from a value a bit higher than the defined capture velocity to a value close to zero.
-----------------	---

<i>Nt=10e3</i>	Number of samples for the time vector for speed calculation. A small number will may lead to atoms not crossing the whole apparatus, while a big one will lead to longer simulation time.
<i>dt=1e-6</i>	Time vector resolution [s]. It is the time hops between one speed calculation and the next one. A high value will lead to a rough curve in atoms deceleration and, maybe, a not realistic calculations as deceleration is supposed to be constant within that time period. Smaller values will increase the CPU consumption. User may change the parameter, but 1 μ s works well for typical slowers. In case of modification, recommendation is not to move far away from this value [0.1 – 2] μ s, and Nt shall be modified consequently.
<i>atoms_initial_z_position=-75</i>	z-position [mm] where atoms start moving towards the slower. It should include all zone where generated B field is not close to zero, otherwise it may lead to unrealistic results.
<i>use_sigma_plus = False</i>	Consider use of additional polarization. In some slowers, although one light polarization is used for the transition, there is some component of other light polarization. Changing this parameter to <i>True</i> will consider the same amount of power affecting atoms by presence of this polarization, typically in zones where B field has matching values with reverse slope.

Next two sections include data needed from the atomic species. Right now, the tool DOZE only includes ^{87}Sr and ^{171}Yb . These parameters can only be changed via the [config.ini](#) file:

[atomic_parameter_sr]	Section title.
<i>m = 86.9089</i>	^{87}Sr mass [u.m.a].
<i>WL_ge = 4.6086212862e-07</i>	Transition wavelength for ^{87}Sr [m].
<i>gamma = 30.24e6</i>	Transition bandwidth for ^{87}Sr [Hz].
<i>mu_eff = -0.9994071129074684</i>	Transition effective magnetic moment in units of Bohr Magnetron [μ_B] for ^{87}Sr .
[atomic_parameter_Yb]	Section title.
<i>m = 170.9363</i>	^{171}Yb mass [u.m.a].
<i>WL_ge = 3.9900005912113637e-07</i>	Transition wavelength for ^{171}Yb [m].
<i>gamma = 28999622.18077425</i>	Transition bandwidth for ^{171}Yb [Hz].
<i>mu_eff = -1.035</i>	Transition effective magnetic moment in units of Bohr Magnetron [μ_B] for ^{171}Yb .

This section includes the resolution of the curve to create and calculate B fields.

[number of points to calculate B]

B_points=1001 Number of points in the deceleration zone for the ideal B field.

B_points_additional=400 Number of additional points before and after the deceleration zone.

This section includes a scaling factor to avoid excessive slowing due to certain B field outside deceleration zone.

[scale_factor_B]

scale_factor_B=1.05 Factor to reduce the B field slope avoiding excessive B field outside deceleration zone stops atoms further than desired. Value 1.05 usually leads to results where V_{fin} is quite close to desired one, with the only need to modify a bit last two magnets positions.

4. STRUCTURE OF THE HDF5 DATA FILE

H5 file is saved when pressing button **Save data files** in a folder with name structure *YYYYMMDD_SavedData* and name format *HH_MM_SS_simulation_data.h5*.

Inside this file user may find most of data used in the current simulation as well as some of the values calculated in execution time. These data is structured in groups like this:

- Atomic_Kinetics: group where datasets with atoms velocities and positions -if calculated- will be stored:
 - Atom velocities $z[m \cdot s^{-1}]$: 2D array. Each row represents the speed evolution of an atom starting at certain speed along time vector of step dt .
 - Atoms positions $z[mm]$: 2D array. Each row represents the position evolution of an atom starting at certain speed along time vector of step dt .
- Field_Profiles: group where dataset with magnetic field B profiles are stored:
 - $B_{y_current}$ [mT]: 1D array. Column represents B field generated by magnets at each point of the z-axis.

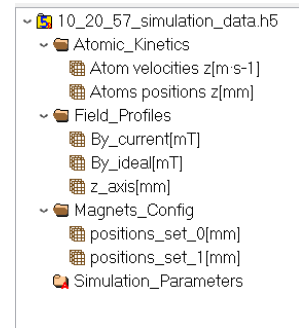


Figure 4.1. Data in hierarchical tree.

- B_{y_ideal} [mT]: 1D array. Column represents ideal B field at each point of the z-axis.
 - z_axis [mm]: 2D array. Matrix where each column represent the x-y-z value of the 3D z-axis where atoms will move and where B field will be computed.
- Magnets_Config: group where datasets with magnets positions are stored:
 - $Positions_set_0$ [mm]: 2D array. Matrix where each column represents the x-y-z value of the position of magnets over ($z > 0$) the vacuum tube.
 - $Positions_set_1$ [mm]: 2D array. Matrix where each column represents the x-y-z value of the position of magnets under ($z < 0$) the vacuum tube.

- Simulation_Parameters: group where single attributes used in the simulation are stored:
 - Atom_species [string], indicates usage of ^{87}Sr or ^{171}Yb .
 - I_max [float] in W/m^2 , indicates maximum intensity provided by laser source.
 - I_sat [float] in W/m^2 , indicates saturation intensity for the transition.
 - LZ [float] in m, deceleration distance for the slower.
 - N_vel [int] in #, number of different velocities to simulate.
 - Npm [int] in #, number of pair of magnets to be user in the simulation.
 - Nt [int] in #, elements of vector time for atoms kinetics.
 - P [float] in W, laser power on pure polarization needed to induce the transition.
 - Tmagz [int] in mT, remanence of magnets used.
 - V_cap [int] in m/s, desired capture velocity.
 - V_fin [int] in m/s, desired final velocity of atoms.
 - WL_ge [float] in m, nominal transition wavelength.
 - atoms_initial_z_position [float] in mm, z-position where atoms start moving towards slower.
 - do_Mhz [float] in MHz, laser detuning.
 - disp [float] in mm, minimum movement on y-position of magnets by spinboxes or during magnets position optimization process.
 - eta [float] in a.u., rate of total power used on the slower.
 - ext_tube_radius [float] in mm, external radius of vacuum tube.
 - gammao [float] in Hz, transition linewidth.
 - ko [float] in m^{-1} , nominal transition wave number.
 - m [float] in kg, atoms mass.
 - mag_diam [float] in mm, magnets diameter.
 - mag_heig [float] in mm, magnets height.
 - min_magnet_distance [float] in mm, minimum distance to the centre of the tube a magnet can be placed, defined by adding external_tube_radius and safety margin.
 - mu_eff [float] in a.u., rate of effective magnetic moment divided by Bohr magneton.
 - s_max [float] in a.u.
 - scale_factor_B [float] in a.u., factor to reduce the B field slope avoiding excessive B field outside deceleration zone stops atoms further than desired.
 - sep_ini [float] in mm, y-distance separation between first magnet (outside deceleration zone) and second (first inside deceleration zone). Positive means the magnet outside deceleration zone is closer to the tube. This distance controls the initial slope of B field in deceleration zone.
 - sep_last [float] in mm, y-distance separation between last magnet (outside deceleration zone) and the one before last (last inside deceleration zone). Positive means the magnet outside deceleration zone is closer to the tube. This distance controls the final slope of B field in deceleration zone and the final velocities of the atoms.
 - use_sigma_plus [bool] in Boolean, indicates if opposite light polarization is present.
 - wo [float] in mm, diameter of light beam waist.
 - zero_cross [float] in number #, number of theoretical magnet where B field crosses zero.

5. TIPS FOR DOZE USAGE

DOZE is not really a commercial tool and its usage may bring some issues. Below are described the most important conflicts that may lead this tool to deviate from its expected behaviour:

- **Number of magnets (pairs):** Less than four doesn't allow the tool to run the algorithm for magnets position optimization as at least two magnets have to appear at each side of the B-field crossing zero. Maximum number is twenty, due to room needed to deploy the spin boxes to move each pair of magnets
- **Detuning:** It is responsible for B-field crossing zero. Selecting a too high or too low one can lead to leaving less than two magnets by the end of the apparatus or to a very high B-field requirement that cannot be accomplished by magnets as the vacuum tube restricts how close they can be.
- **Number of velocities to simulate the atomic kinetics:** A very high number will lead to a high CPU consumption or time to made calculations. Minimum is $N_{vel} = 2$ and will show the capture velocity and its double which will not show really the behaviour of the slower. For initial calculations $N_{vel} = 5$ is a good initial approximation while a more detailed analysis will require around 10.
- **Deceleration length:** There is a minimum value the slower can be if the laser power is very high. It is not possible to decelerate atoms from about 400 m/s to 30-40 m/s in less than 12-15 cm. Select a reasonable length. An indicative table ([Table 2.1](#)) is shown in [chapter 2](#) at the end of section [Atomic kinetics simulation](#).
- **Remanence.** Available Nd magnets of the sizes considered can perform a remanence of around 1300 mT. Selecting much greater remanence values can lead to unrealistic results.

6. PYTHON LIBRARIES VERSIONS

As most cases in python, libraries must match those used within the development. The most important are:

- h5py: 3.15.1
- magpylib: 4.5.1
- matplotlib: 3.10.7
- numpy: 2.3.5
- plotly: 6.5.0
- PyQt5: 5.15.11
- scipy: 1.16.3

Other libraries used, related or depending from previous ones, are:

- Altgraph: 0.17.5
- Colorama: 0.4.6
- Contourpy: 1.3.3
- Cycler: 0.12.1
- Fonttools: 4.60.1
- kiwisolver: 1.4.9
- mpmath: 1.3.0
- narwhals: 2.12.0

- packaging: 25.0
- pefile: 2024.8.26
- pillow: 12.0.0
- pip: 25.3
- pyinstaller: 6.17.0
- pyinstaller-hooks-contrib: 2025.10
- pyparsing: 3.2.5
- PyQt5-Qt5: 5.15.2
- PyQt5_sip: 12.17.1
- python-dateutil: 2.9.0.post0
- pywin32-ctypes: 0.2.3
- setuptools: 80.9.0
- six: 1.17.0
- sympy: 1.14.0
- wheel: 0.45.1

Nevertheless, a file with the of environment libraries used is provided to be imported in any equipment with their proper version.

7. LICENSE AND DISCLAIMER

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DOZE is a research tool intended for academic and experimental physics contexts.