WimPyDD: an object–oriented Python code for the calculation of WIMP direct detection signals

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Abstract. We introduce WimPyDD, a modular, object–oriented and customizable Python code that calculates accurate predictions for the expected rates in Weakly Interacting Massive Particle (WIMP) direct–detection experiments within the framework of Galilean–invariant non–relativistic effective theory in virtually any scenario, including inelastic scattering, an arbitrary WIMP spin and a generic WIMP velocity distribution in the Galactic halo. WimPyDD exploits the factorization of the three main components that enter in the calculation of direct detection signals: i) the Wilson coefficients that encode the dependence of the signals on the ultraviolet completion of the effective theory; ii) a response function that depends on the nuclear physics and on the main features of the experimental detector (acceptance, energy resolution, response to nuclear recoils); iii) a halo function that depends on the WIMP velocity distribution and that encodes the astrophysical inputs. In WimPyDD these three components are calculated and stored separately for later interpolation and combined together only as the last step of the signal evaluation procedure. This makes the phenomenological study of the direct detection scattering rate with WimPyDD transparent and fast also when the parameter space of the WIMP model has a large dimensionality.
1 Introduction

Weakly Interacting Massive Particles (WIMPs) provide the most popular candidates for the Cold Dark Matter (CDM) that is known from gravitational measurements to constitute about 25% of the density of the Universe, is concentrated in Galaxies like the Milky Way and is required in any model of Galaxy formation. WIMPs have feeble interactions of the Weak or Super-Weak type with ordinary matter that allow them to thermalize in the early Universe and that can predict the correct relic density through the thermal decoupling mechanism. A worldwide experimental effort is under way to observe such interactions. In direct detection
(DD) experiments WIMP-nucleus scattering events are searched for in solid-state or liquid-state detectors in underground laboratories protected by cosmic rays.

The calculation of DD signals depends on particle physics, nuclear physics and astrophysics inputs. Moreover, in order to obtain realistic predictions, experimental features such as the energy resolution and the efficiency of the detector and the specific response of the target material to nuclear recoils (quenching, light yield) are required. In the present paper we introduce WimPyDD, a customizable, object-oriented Python code that allows to handle all such different inputs in a modular way to obtain accurate predictions for the expected signal in WIMP DD experiments in virtually any theoretical scenario. Before its present release WimPyDD was extensively tested in several publications [1–7].

In particular, WimPyDD is specifically designed to calculate WIMP DD signals in generalized scenarios, whose relevance in present research is twofold: first, accelerator physics has not provided so far any information or hint about the physics beyond the standard model that must be related to the Dark Matter (DM) particle, so that model-independent approaches have become increasingly popular to interpret Dark Matter search experiments. Moreover, the incoming WIMP flux in DD experiments depends on the velocity distribution of such particles in the halo of our Galaxy, which is in principle not known.

Since the DD process is non-relativistic (NR) the WIMP-nucleon interaction can be parameterized with an effective Hamiltonian $\mathcal{H}$ that complies with Galilean symmetry. The effective Hamiltonian $\mathcal{H}$ to zero-th order in the WIMP-nucleon relative velocity $\vec{v}$ and momentum transfer $\vec{q}$ has been known since at least Ref. [8], and consists of the usual spin-dependent (SD) and spin-independent (SI) terms. To first order in $\vec{v}$, the effective Hamiltonian $\mathcal{H}$ has been systematically described in [9, 10] for WIMPs of spin 0 and 1/2, and less systematically described in [11, 12] for WIMPs of spin 1 and in [13] for WIMPs of spin 3/2. Recently in [14] the NR effective Hamiltonian for WIMP-nucleus scattering has been extended to include WIMPs of arbitrary spin $j_\chi$. In Ref. [14] $\mathcal{H}$ is written in a complete base of rotationally invariant operators organized according to the rank of the $2j_\chi + 1$ irreducible operator products of up to $2j_\chi$ WIMP spin vectors. In particular, for a WIMP of spin $j_\chi$ a base of $4 + 20j_\chi$ independent operators is obtained that can be matched to any high-energy model of particle dark matter, including elementary particles and composite states. WimPyDD incorporates the formalism of Ref. [14], allowing to introduce an effective Hamiltonian for generic WIMP spin $j_\chi$ and Wilson coefficients that are arbitrary functions of external parameters and of the momentum $q$ transferred in the scattering process.

To calculate expected signals WimPyDD makes full use of the fact that DD signals can be written as the convolution of three factorized components: i) the Wilson coefficients, that depend on arbitrary external parameters $w_i$; ii) a response function $R$, that depends on the nuclear physics and on the features of the experimental detector (acceptance, energy resolution, response to nuclear recoils); iii) a halo function $\eta$, that depends on the WIMP velocity distribution and that encodes the astrophysical inputs [15, 16]. In WimPyDD these three components are calculated separately and combined together only at the last step of the signal evaluation procedure. In particular the response functions $R$ and the halo function $\eta$ are calculated and stored for later interpolation using parameterizations in terms of the recoil energy and the WIMP incoming velocity, respectively, that do not depend on the scattering kinematics (i.e. on the WIMP mass $m_\chi$ and on the mass splitting $\delta$ in the case of inelastic scattering (IDM) [17]). This makes the phenomenological study of the DD scattering rate

\[ ^1 \text{In IDM a DM particle of mass } m_\chi \text{ interacts with atomic nuclei exclusively by either up-scattering to a heavier state with mass } m_\chi + \delta \text{ or down-scattering to a lighter state with mass } m_\chi - \delta \text{ (this latter case is} \]
transparent and fast also when the parameter space \((m_\chi, \delta, w_i)\) has a large dimensionality.

The paper is organized as follows: in Section 2 we introduce the theoretical background of WIMP nuclear scattering and show the factorizations used by WimPyDD to optimize the expressions used for the numerical evaluation of the signals; in Section 3 we introduce the code. We explain its installation in 3.1; introduce the signal routines in 3.2 and the classes required to use them in 3.3. At the core of how WimPyDD works are the integrated response functions \(R\), which at the stage of signal evaluation are below the lid and invisible to the user. However knowing how such response functions are handled by WimPyDD is crucial for the user to run the code properly and to exploit its optimizations, so Section 3.4 provides a detailed discussion of this issue, with a particular focus on the aspect of how Wilson coefficients that depend on the exchanged momentum are implemented. In Section 3.5 we illustrate the use of WimPyDD through some examples. Several details needed to understand the code are provided in the Appendices: Appendix A integrates Section 2 with detailed expressions for the scattering rates and the response functions; Appendix B illustrates the two alternative bases for the operators of the effective Hamiltonian that can be used in the code; in Appendix C a detailed explanation of how to initialize a DD experimental set-up in WimPyDD is given; Appendix D explains how to add new nuclear targets and their response functions; Appendix E explains how to calculate the halo function; finally, Appendix F provides a summary of the WimPyDD components and their correspondence to the theoretical formulas introduced in Section 2 and in Appendix A.

## 2 WIMP direct detection scattering rate

Formulas for the calculation of expected WIMP DD signals have been available in the literature for a long time (see for instance [18]). However to optimize their numerical evaluation WimPyDD makes explicit use of the factorization among Wilson coefficients, the halo function and the experimental response functions, and exploits a parameterization of the latter that is independent on the WIMP mass \(m_\chi\) and on the mass splitting \(\delta\). Since the relevant expressions are not available in the literature in this Section we outline them (additional details are provided in A).

The expected number of events in a WIMP DD experiment in the interval of visible energy \(E'_1 \leq E' \leq E'_2\) can be cast in the form [16]:

\[
R_{[E'_1, E'_2]}(t) = \frac{\rho_\chi}{m_\chi} \int_{v_{T^*}}^{\infty} \sum_T dv R_{T; [E'_1, E'_2]}(v) \eta(v, t),
\]

with \(\rho_\chi\) the WIMP local density in the neighborhood of the Sun, \(m_\chi\) the WIMP mass,

\[
v_{T^*} \equiv \begin{cases} \sqrt{\frac{2\delta}{\mu_\chi T}}, & \text{if } \delta > 0 \\ \sqrt{\frac{\delta}{\mu_\chi T}}, & \text{if } \delta \leq 0 \end{cases}
\]

and the sum is over the nuclear targets \(T\). In the expression above:

\[
\eta(v, t) = \int_v^{\infty} \frac{f(v', t)}{v'} \, dv', = \int_v^{\infty} \frac{f(v', t)}{v'} \, dv',
\]

referred to as exothermic DM). WimPyDD can handle both cases.
is a halo function that depends on the WIMP speed distribution \( f(v, t) \equiv 1/(4\pi) \int d\Omega v'^2 f(v', t) \) (present DD experiments are not sensitive to the incoming direction of the WIMP), while \( R_{[E'_1, E'_2]}^{T}(v) \) is a response function that depends on the WIMP–target interaction and on the features of the detector. If the speed distribution is written in terms of a superposition of \( N_s \) streams:

\[
f(v, t) = \sum_{k}^{N_s} \lambda_k(t) \delta(v - v_k), \tag{2.4}
\]

the halo function becomes:

\[
\eta(v, t) = \sum_{k=1}^{N_s} \frac{\lambda_k(t)}{v_k} \Theta(v_k - v) = \sum_{k=1}^{N_s} \delta \eta_k(t) \Theta(v_k - v), \tag{2.5}
\]

and in Eq. (2.1) one has the following factorization:

\[
R_{[E'_1, E'_2]}^{T}(t) = \frac{\rho X}{m_X} \sum_{k=1}^{N_s} \delta \eta_k(t) \int_{v_{T^*}}^{v_T} \sum_{T} dv R_{T,[E'_1, E'_2]}(v). \tag{2.6}
\]

Most DD experiments put upper bounds on the time average of \( R_{[E'_1, E'_2]}^{T}(t) \):

\[
S_{[E'_1, E'_2]}^{(0)} = \frac{1}{T_0} \int_{0}^{T_0} R_{[E'_1, E'_2]}^{T}(t) dt, \tag{2.7}
\]

(with \( T_0 = 1 \) year) while dedicated large-mass detectors such as those of DAMA [19], COSINE [20] or ANAIS [21] are sensitive to the yearly modulation effect ensuing from the time dependence of the Earth velocity \( \vec{v}_E(t) \) due to its rotation around the Sun. In particular, the latter measure the cosine transform of \( R_{[E'_1, E'_2]}^{T}(t) \):

\[
S_{[E'_1, E'_2]}^{(1)} = \frac{2}{T_0} \int_{0}^{T_0} \cos \left[ \frac{2\pi}{T_0} (t - t_0) \right] R_{[E'_1, E'_2]}^{T}(t) dt, \tag{2.8}
\]

with \( t_0 = \text{June, 2}\text{nd} \). Using Eq.(2.1) in Eq.(2.7) and Eq.(2.8) one gets:

\[
S_{[E'_1, E'_2]}^{(0,1)} = \int_{v_{T}}^{\infty} \sum_{T} dv R_{T,[E'_1, E'_2]}(v) \eta^{(0,1)}(v), \tag{2.9}
\]

\[
\eta^{(0)}(v) = \frac{1}{T_0} \int_{0}^{T_0} \eta(v, t), \tag{2.9}
\]

\[
\eta^{(1)}(v) = \frac{2}{T_0} \int_{0}^{T_0} \cos \left[ \omega (t - t_0) \right] \eta(v, t), \quad \omega = \frac{2\pi}{T_0}. \tag{2.10}
\]

where \( \mu_{X T} \) is the WIMP–target reduced mass. This implies that Eq. (2.6) can be directly used to calculate \( S_{[E'_1, E'_2]}^{(0)} \) and \( S_{[E'_1, E'_2]}^{(1)} \), provided that the substitution \( \delta \eta_k(t) \rightarrow \delta \eta_k^{(0,1)} \), with:

\[
\eta^{(0,1)}(v) = \sum_{k=1}^{N_s} \delta \eta_k^{(0,1)} \Theta(v_k - v). \tag{2.11}
\]

is made.
In Appendix A (see Eq. (A.18)) it is shown that the integral on the right–hand side of Eq. (2.6) takes the form:

\[
\int_{v_T^*}^{v_i} \sum_T dV \mathcal{R}_{T,[E_1',E_2']}(v) = \\
\int_{E_R^{\text{min}}(v_i)}^{E_R^{\text{max}}(v_i)} dE_R \left[ \mathcal{R}_{T,[E_1',E_2']}(E_R) + \mathcal{R}_{T,[E_1',E_2']}(E_R) (v_i^2 - v_{T,min}^2(E_R)) \right],
\]

(2.12)

(see Eqs. (A.14, A.15) for the explicit expressions of \(\mathcal{R}_{T,[E_1',E_2']}\)). In Eq. (2.12):

\[
\quad v_{T,min}(E_R) = \frac{1}{\sqrt{2 m_T E_R}} \left| \frac{m_T E_R}{\mu_{\chi T}} + \delta \right|,
\]

(2.13)

is the minimal speed an incoming WIMP needs to have in the target reference frame to deposit energy \(E_R\) (with \(m_T\) the nuclear target and \(\delta\) the mass splitting in case of inelastic scattering). In the same equation:

\[
\quad E_R^{\text{min,max}}(v) = \left[ \frac{\mu_{\chi T}}{2 m_T} \left( v \mp \sqrt{v^2 - v_{T^*}^2} \right) \right]^2,
\]

(2.14)

with \(v_{T^*}\) given in Eq. (2.2).

The most general WIMP-nucleus interaction complying with Galilean symmetry can be parameterized with an effective Hamiltonian \(\mathcal{H}\) of the form [9–12, 14]:

\[
\quad \mathcal{H}(w_i, q) = \sum_{\tau=0,1} \sum_j c_j^\tau (w_i, q) \mathcal{O}_j(q) t^\tau.
\]

(2.15)

In the equation above we have explicitly written the dependence of the effective Hamiltonian on some parameters \(w_i\) (which can include the WIMP mass \(m_\chi\) and the mass splitting \(\delta\)) arising from the matching of the Wilson coefficients of the low–energy effective theory to its ultraviolet completion, and on the transferred momentum \(q\) (for instance through a propagator). All \(\mathcal{O}_j\) operators for \(j_\chi \leq 1/2\), and some for \(j_\chi = 1\) are listed in Table 1. Moreover, in Eq. (2.15), \(t^0 = 1\), \(t^1 = t_3\) denote the 2 \(\times\) 2 identity and third Pauli matrix in the nucleon isospin space, respectively, and the isoscalar and isovector Wilson coefficients coupling \(c_j^0\) and \(c_j^1\) are related to those to protons and neutrons \(c_j^p\) and \(c_j^n\) by \(c_j^p = (c_j^0 + c_j^1)/2\) and \(c_j^n = (c_j^0 - c_j^1)/2\).

If the scattering process is driven by the Hamiltonian of Eq. (2.15) the functions \(\mathcal{R}^{\tau}_T[E_1',E_2']\) in Eq.(2.12) are quadratic in the Wilson coefficients of the effective theory, that can be factored out:

\[
\quad \mathcal{R}^{\tau}_T[E_1',E_2'](E_R) = \sum_{j,k} c_j^\tau (w_i, q_0) c_k^{\tau'} (w_i, q'_0) \left[ \mathcal{R}^i_T[E_1',E_2'] \right]_{jk} (E_R). \quad (2.16)
\]

In the expression above \(q_0, q'_0\) are arbitrary momentum scales in the case when the Wilson coefficients \(c_j^\tau, c_k^{\tau'}\) have an explicit dependence on \(q\). Using in Eq. (2.12) the explicit expression of the square of \(v_{T,min}(E_R)\):
and defining the integrated response functions:

\[
\left[ \mathcal{R}_{T,[E_1',E_2']}^{i}(E_R) \right]^{\tau\tau'}_{jk}(E_R) = \int_0^{E_R} dE_R' \left[ \mathcal{R}_{T,[E_1',E_2']}^{i}(E_R') \right]^{\tau\tau'}_{jk}(E_R'), \quad i = 0, 1
\]

\[
\left[ \mathcal{R}_{T,[E_1',E_2']}^{1F}(E_R) \right]^{\tau\tau'}_{jk}(E_R) = \int_0^{E_R} dE_R' E_R' \left[ \mathcal{R}_{T,[E_1',E_2']}^{1F}(E_R') \right]^{\tau\tau'}_{jk}(E_R'),
\]

\[
\left[ \mathcal{R}_{T,[E_1',E_2']}^{1E^{-1}}(E_R) \right]^{\tau\tau'}_{jk}(E_R) = \int_0^{E_R} dE_R' \frac{1}{E_R'} \left[ \mathcal{R}_{T,[E_1',E_2']}^{1E^{-1}}(E_R') \right]^{\tau\tau'}_{jk}(E_R'),
\]

the predicted rate for both the time-averaged and the yearly modulated signals can then be written as:

\[
S^{(0,1)}_{[E_1',E_2']} = \frac{\rho_\chi}{m_\chi} \sum_{k=1}^{N_\chi} \delta \eta^{(0,1)}_k \times \sum_{T} \sum_{ij} \sum_{\tau\tau'} c_j^c(w_i,q_0)c_k^c(w_i,q_0)
\]

\[
\left\{ \left[ \mathcal{R}_{T,[E_1',E_2']}^{0}(E_R) \right]^{\tau\tau'}_{jk}(E_R) + \left( \frac{v_k^2}{c^2} - \frac{\delta}{\mu T} \right) \left[ \mathcal{R}_{T,[E_1',E_2']}^{1}(E_R) \right]^{\tau\tau'}_{jk}(E_R) \right\}_{E_R}^{E_R^{max}(v_k)} - \frac{m_T}{2\mu T} \left[ \mathcal{R}_{T,[E_1',E_2']}^{1}(E_R) \right]^{\tau\tau'}_{jk}(E_R) - \frac{\delta^2}{2m_T} \left[ \mathcal{R}_{T,[E_1',E_2']}^{1E^{-1}}(E_R) \right]^{\tau\tau'}_{jk}(E_R) \right\}_{E_R}^{E_R^{min}(v_k)},
\]

where \( \{ f(E_R) \}_{E_R}^{E_R^{max}} \equiv f(E_2) - f(E_1) \). The expression above is the master formula used by WimPyDD to calculate expected rates. As anticipated, it exploits explicitly the factorization of the the Wilson coefficients \( c_j^c \), the response functions \( \left[ \mathcal{R}_{T,[E_1',E_2']}^{a}(E_R) \right]_{jk}^{\tau\tau'} \) and of the the halo functions \( \delta \eta^{(0,1)}_k \). Crucially, in Eq. (2.19) the only dependence on \( m_\chi \) and \( \delta \) is through \( E_R^{min,max}(v_k) \) (see Eq. (2.14)). In particular, the numerical calculation of the integrated response functions \( \left[ \mathcal{R}_{T,[E_1',E_2']}^{a}(E_R) \right]_{jk}^{\tau\tau'} \) can be time consuming since they require the evaluation of double integrals. However, they depend only on the single external argument \( E_R \). The main strategy used by WimPyDD to speed up the calculation of the rates is to tabulate each \( \left[ \mathcal{R}_{T,[E_1',E_2']}^{a}(E_R) \right]_{jk}^{\tau\tau'} \) as a function of \( E_R \) for later interpolation. As already mentioned such tables do not depend on the WIMP mass \( m_\chi \) and on the mass splitting \( \delta \), that only enter in the mapping between the \( v_k \) values and the energies \( E_R^{max}(v_k) \) and \( E_R^{min}(v_k) \) at which the response functions in the tables are interpolated.
Figure 1. Main structure of WimPyDD. Diamond–shaped elements indicate the input from the user, oval shapes contain classes and rectangles represent functions. Three final outputs are possible: the differential cross section \( \frac{d\sigma}{dE_R} \) defined in Eq. (A.5), the differential rate \( \frac{dR}{dE_R} \) defined in Eq. (A.4) and the integrated expected rate \( S_{[E'_1,E'_2]}^{(0,1)} \) given in Eqs. (2.7-2.8).

3 The WimPyDD code

WimPyDD is a modular, customizable and flexible code written in Python 3.7 that allows to implement the formulas outlined in Section 2 with a full control on each input. The versatility of the code is at the expense of some degree of complexity. However most functionalities can be used with default choices, so the beginner can start producing sensible output with just a few simple calls. The present introduction to the code will mostly describe default features, with a few mentions to possible generalizations. More details about WimPyDD’s functionalities and example files are available at:

\[
\text{https://wimpydd.hepforge.org}
\]

where also the code and additional explanations are available. Also use the \texttt{help()} function from the Python command line to get detailed information about any component of the code.

The structure of the code is summarized in Fig. 1. In such figure diamond–shaped elements indicate the input from the user, oval shapes contain classes and rectangles represent functions. Three final outputs are possible, the differential cross section \( \frac{d\sigma}{dE_R} \) defined in Eq. (A.5), the differential rate \( \frac{dR}{dE_R} \) defined in Eq. (A.4) and the integrated expected rate \( S_{[E'_1,E'_2]}^{(0,1)} \) given in Eqs. (2.7-2.8).

\[3\] Notice that a different response function must be calculated for each target, energy bin, \( c'_i c'_j \) combination and \( a = 0, 1, 1E, 1E^{-1} \).
expected rate $\mathcal{S}^{(0,1)}_{[E_1',E_2']} \approx \frac{\partial \sigma}{\partial \eta} |_{1}^{\infty}$ given in Eq. (2.19), that includes the detector’s response: the calculation of $(d\sigma/dE_R)_T$ requires the minimal set of inputs, the nuclear target(s) $T$ and an effective Hamiltonian $\mathcal{H}$; in addition to them, to evaluate $(dR/dE_R)_T$ the halo function $\eta(v)$ is required; finally the evaluation of the integrated rate $R_{[E_1',E_2']} \approx \frac{\partial R}{\partial E_R}$ requires to fix a specific experimental set-up. A simple routine that calculates exclusion plots in the familiar mass–cross section plane is also provided.

3.1 Installation

To install the latest version of WimPyDD type:

```
git clone https://phab.hepforge.org/source/WimPyDD.git
```
in the working directory, or download the code from WimPyDD’s homepage. This will create a folder WimPyDD. All the libraries required by the code are standard, such as matplotlib, numpy, scipy and pickle. To import WimPyDD type something like:

```
import WimPyDD as WD
```

3.2 Signal routines

To calculate the differential cross section $(d\sigma/dE_R)_T$ (in cm$^2$/keV) use:

```
WD.dsigma_der(element_obj,hamiltonian_obj,mchi,v,
er,**args)
```

with $m_{\chi}$ the WIMP mass $m_{\chi}$ in GeV, $v$ the WIMP incoming speed in km/sec, $er$ the recoil energy in keV, and where `element_obj` defines a nuclear target $T$ (see Section 3.3.1) while `hamiltonian_obj` defines an effective Hamiltonian (see Section 3.3.3).

To evaluate the differential rate $dR/dE_R$ use the routine:

```
WD.diff_rate(target_obj,hamiltonian_obj,mchi,
energy,vmin,delta_eta, **args)
```

`target_obj` is either a single element or a combination of elements with stoichiometric coefficients (see Section 3.3.2). The output of `diff_rate` is in events/kg/day/keV if the `exposure` argument is not passed (its default value is 1 kg day). The argument `energy` is in keV and is interpreted as the electron-equivalent energy $E_{ee}$ for the elements that have the `quenching` attribute, otherwise as the recoil energy $E_R$ (see Eq. (A.2) and below for the definitions of $E_{ee}$, $E_R$ and of the quenching factor). Quenching is an attribute of the experimental set-up, so can be added to a target using the `experiment` class (see Section 3.3.1 and, for a specific example, Section 3.5.1).

Finally, `vmin` and `delta_eta` are two arrays containing the $v_k$ and $\delta \eta_k^{(0,1)}$ of Eq. (2.11) in km/s and (km/s)$^{-1}$, respectively (WimPyDD provides the routine `streamed_halo_function` to calculate them, see Appendix E).

In order to calculate the integrated rate of Eq. (2.1) including the detector’s response, use:
where \texttt{exp_obj} is instantiated by the \texttt{experiment} class and contains all the required information about the experimental set-up, including the energy bins where the rate is integrated (see Appendix C). The routine returns two arrays with the centers of the bins and the corresponding expected rates calculated using Eq. (2.19).

In all WimPyDD routines by default $\delta=0$ and $j_\chi=1/2$; such values can be changed using the arguments \texttt{delta} and \texttt{j_chi}. Moreover in all signal routines the parameters entering the Wilson coefficients of the effective Hamiltonian are passed through the keyworded arguments list \texttt{**args}. Additional default-valued arguments allow to tune the output and behavior of all WimPyDD routines, type \texttt{help} from the Python command line to learn more. Explicit examples of the use of the signal routines are provided in Section 3.5.

### 3.3 Main classes

#### 3.3.1 Element

**Main attributes:** a (array with isotopic atomic numbers), \texttt{abundance} (array of isotopic natural abundances), \texttt{quenching} (quenching factor - only present if the element belongs to the target of an \texttt{experiment} object), \texttt{func_w} (array of isotopic nuclear response functions $W_{l\tau'}$), \texttt{isotopes} (array with list of isotopes), \texttt{mass} (array with isotope masses), \texttt{name} (full name of element), \texttt{nt_kg} (array with isotopic numbers of targets per kg), \texttt{spin} (array with isotope spins), \texttt{symbol} (element symbol), \texttt{z} (atomic number).

WimPyDD provides a list of 20 pre-defined elemental targets that can be shown with the command:

```python
WD.list_elements()
WD.Al WD.Ar WD.C WD.Ca WD.F WD.Fe
WD.Ge WD.H WD.He WD.I WD.Mg WD.N
WD.Na WD.Ne WD.Ni WD.O WD.S WD.Si
WD.W WD.Xe
```

To implement additional elements see Appendix D.

#### 3.3.2 Target

**Main attributes:** \texttt{element} (array with list of elements), \texttt{formula} (molecular formula), \texttt{mass} (total mass), \texttt{n} (array with stoichiometric coefficients), \texttt{nt_kg} (array with number of targets per kg for each element of the target).

A nuclear target can by any combination of \texttt{element} and/or \texttt{target} objects with stoichiometric coefficients. For instance, to define an octafluoropropane ($C_3F_8$) target:

```python
C3F8=3*WD.C+8*WD.F
```

The output of any linear combination of \texttt{element} and/or \texttt{target} objects is a \texttt{target} object. The same result is obtained by directly invoking the \texttt{target} class with a string argument containing the element names and the stoichiometric coefficients, i.e.:
It is at this stage that, in order to correctly parse the input string, the element string names are required to begin with a capital letter (i.e. `WD.target('CaWO4')` is parsed correctly, while `WD.target('cawo4')` is not). The `target` class needs also to be invoked for a pure elemental target (the same result is obtained by multiplying an `element` object times 1):

```python
germanium_target1=WD.target('Ge')
germanium_target2=1*WD.Ge
```

Notice that inside a `target` object `element` instantiations are sensitive to the environment. For instance, the `element.nt_kg` attribute contains the number of target per unit mass $N_T$ for each element (see for instance Eq. (A.3)). This quantity is different if it refers to one kg of carbon or fluorine, or if it refers to 1 kg of $C_3F_8$:

```python
print(WD.F.nt_kg)
[3.16842105e+25]
print(c3f8.element[1])
fluorine, symbol F, atomic number 9, average mass 17.689, 1 isotopes.
print(c3f8.element[1].nt_kg)
[2.56125255e+25]
```

### 3.3.3 Effective Hamiltonian

**Main attributes:** `coeff_squared_list` (list of operators products in scattering amplitude), `couplings` (list of effective operators), `wilson_coefficients` (dictionary with effective operators and Wilson coefficients).

A specific effective Hamiltonian Eq.(2.15) is set–up by a list of interaction operators and their corresponding Wilson coefficients. In WimPyDD this is done by instantiating the class `eft_hamiltonian`, which takes two arguments: a string containing a name of user’s choice for the Hamiltonian and a Python dictionary with the operators and the Wilson coefficients:

```python
wc={n1: func1 , n2: func2, ... }
hamiltonian_obj=WD.eft_hamiltonian('name',wc)
```

In WimPyDD two alternative sets of non–relativistic effective operators can be used. The keys $n_1, n_2, ...$ of the dictionary `wc` identify such operators and are integer numbers for the base of operators introduced in [9, 10] or tuples $(X,s,l)$ for the alternative base introduced in [14]. Further information on the allowed choices for $n_1, n_2, ...$ is provided in Appendix B.

In the same dictionary `func1(par1,par2,...)`, `func2(par1,par2,...)` are functions of arbitrary parameters $par1, par2, ...$ that can include $m_\chi, \delta$ and $q$. They return two-dimensional arrays (or lists) containing the Wilson coefficients $c_j^0, c_j^1$ in GeV$^{-2}$:

```python
def func1(w1,w2,...,mchi,...,delta,...,q):
    ...
    return [c0,c1]```
3.3.4 Experiment

Main attributes: data (list of energy bins - can contain the upper bounds used by mchi_vs_exclusion routine), efficiency (efficiency function), exposure (exposure - can be a list with a different exposure for each energy bin), name (name of experiment - corresponds to the name of the folder with the experimental information), resolution (energy resolution function), response_functions (dictionary with tables of integrated response functions), target (experimental target).

In order to include the response of the detector the wimp_dd_rate routine requires the integrated response functions $\bar{R}_{aT}[E_{1}',E_{2}']^{\tau\tau'}$ of Eq. (2.18), whose calculation needs information on the experimental set-up: the target, the energy bins, the energy resolution, the efficiency, the quenching factors, the exposure. All such information can be collected in a single Python object by using the class experiment:

```python
exp_obj=WD.experiment(name='exp')
```

that loads it from the folder WimPyDD/Experiments/exp in the user’s working directory (a detailed explanation on how to initialize such directory is provided in Appendix C).

For the effective Hamiltonian hamiltonian_obj, the experimental set up experiment_obj and WIMP spin $j$ the response functions are stored in the dictionary entry:

```python
exp_obj.response_functions=
{(hamiltonian_obj,j):r}
```

by the instruction:

```python
WD.load_response_functions(experiment_obj,
hamiltonian_obj, j)
```

The values $r$ of such dictionary are tuples containing the tables of the response functions. The same tables are also saved in the folder:

(WimPyDD/Experiments/exp/Response_functions/)

(see Section 3.4 for more details). If such folder already contains the tabulated response functions load_response_functions skips the calculation and directly loads them. The function wimp_dd_rate automatically calls load_response_functions if the required response functions are not in the exp_obj.response_functions dictionary.

3.4 Handling the response functions set

An important feature of WimPyDD is that for a given experimental set-up it allows to use the same pool of response functions to study the WIMP parameters space of different effective Hamiltonians. In particular the dependence of signals on a specific theoretical model is factorized in the Wilson coefficients $c_{j}'$, while for all possible combinations $c_{j}'c_{k}'$ the remaining information (nuclear physics + experimental) is stored in the response functions $[\bar{R}_{aT}[E_{1}',E_{2}'][E_{R}]]_{jk}'$. This means that the calculation of signals for different Hamiltonians
instantiated by `WD.eft_hamiltonian` can share the same set of response functions. Whether this is done or not can be decided by the user, and to do it properly requires to know a few more details on how WimPyDD handles them.

For a specific Wilson coefficients dictionary `wc` the `WD.eft_hamiltonian` class stores in the attribute `coeff_squared_list` a lists of all the possible contributions to the squared amplitude, including interferences, which is then used by `WD.load_response_function` to save or load the corresponding response functions. In particular, the names of the files where the response functions are stored is constructed from the keys of `wc`.

For instance, if the two following Hamiltonians `h1` and `h2` are defined, with the functions `func1(w1,w2)`, `func2(w3,w4)`, `func3(w5,w6)` of arbitrary parameters `w1,w2,w3,w4,w5,w6` parameterizing their sets of Wilson coefficients:

```python
h1=WD.eft_hamiltonian('h1', {1: func1, 3: func2})
h2=WD.eft_hamiltonian('h2', {1: func3})

print(h1)
Hamiltonian name:h1
Hamiltonian:func1(w1, w2)* O_1+func2(w3, w4)* O_3
Squared amplitude contributions:
O_1*O_1, O_3*O_1, O_3*O_3

print(h2)
Hamiltonian name:h2
Hamiltonian:func3(w5, w6)* O_1
Squared amplitude contributions:
O_1*O_1
```

the instructions:

```python
xenon1t=WD.experiment('xenon1t')
WD.load_response_functions(xenon1t,h1, j_chi=0.5)
```

save (or load, if already existing) the following set of response functions:

```
c1_c1.npy
c3_c1.npy
c3_c3.npy
```

in the directory `WimPyDD/Experiments/xenon1t/Response_functions/spin_1_2`, while:

```python
WD.load_response_functions(xenon1t,h2, j_chi=0.5)
```

will load

```
c1_c1.npy
```

from the same directory. So `h1` and `h2` will share the same set of response functions contained in `c1_c1.npy`, because they both contain the \(O_1\) operator. This can optimize the calculations saving computing time but must be handled carefully in the case of Wilson coefficients with an explicit momentum dependence. In fact, suppose that the third effective Hamiltonian `h3` is defined:
with \(\text{func}4(w7,q)\) a function that depends explicitly on the transferred momentum \(q\). In this case even if \(h1\) and \(h3\) share the same operator \(O_3\) they do not share the same set of integrated response functions, because the explicit dependence on \(q\) of the Wilson coefficient in \(h3\) implies a different energy dependence in the integrals of Eqs. (2.18). The way WimPyDD handles a Hamiltonian term of the type \(\sum_\tau c^\tau_n(q)O_n(q) t^\tau\) is to factorize the Wilson coefficient at some momentum scale \(q_0\) (see Eq. (2.16)) and treat the the remaining part \(O'_n \equiv c^\tau_n(q)/c^\tau_n(q_0)O_n\) as an operator different from \(O_n\). Crucially, by adding an explanatory string \(\text{string}\) to the the keys of the Wilson coefficient dictionary the user can have full control on which files the response functions of \(O_n\) and \(O'_n\) are saved in. In particular when the base of operators of Ref. [9, 10] is used the integer \(n\) can be substituted by the tuple \((n,\text{string})\), while in the case of the operator base of Ref. [14] the tuple \((X,s,l)\) can be extended to \((X,s,l,\text{string})\).

So in the example above the tuple \((3,'q\_dep')\) is used instead of the simple integer 3, so that the corresponding response functions are saved in the file:

\[
c3\_q\_dep\_c3\_q\_dep.npy
\]

and are not confused with those of \(h1\). Combinations such as:

\[
('Sigma',1,1,'meson\_propagator')
(5,'q\_2\_6\_matching')
\]

are legal options for the coupling keys in the dictionary, leading to the following names of the output files where the tables of the integrated response functions are saved:

\[
c_{Sigma\_1\_1\_meson\_propagator}\_c_{Sigma\_1\_1\_meson\_propagator}.npy
c_{5\_q\_2\_6\_matching}\_c_{5\_q\_2\_6\_matching}.npy
\]

Interferences among different operators \(O'_n\) and \(O_n\) originated from the same \(n\) are automatically included and the corresponding response functions are calculated and saved, or loaded:
In summary, WimPyDD allows to share the same set of response functions for different theoretical scenarios, but it is up to the user to do that appropriately by carefully managing the key names in the Wilson coefficient dictionaries of each `WD.eft_hamiltonian` object.

### 3.5 Examples

In the present Section we introduce the potentialities of WimPyDD by showing some explicit examples.

#### 3.5.1 Differential rate

For this example let’s set up the following effective Hamiltonian:

\[
H = c_0^0 O_1 t^0 + c_1^1 O_1 t^1 = \frac{1}{M^2} [(1 + r)O_1 t^0 + (1 - r)O_1 t^1],
\]

that depends on the two parameters \(M\) and \(r\), that parameterize the WIMP–proton coupling \(c_p^0 = 1/M^2\) and the ratio between the WIMP–proton and the WIMP-neutron coupling \(r = c_n/c_p\). This is implemented by:

```python
wc={1: lambda M, r=1 : [(1.+r)/M**2, (1-r)/M**2] }
SI=WD.eft_hamiltonian('SI',wc)
```

In the instruction above the function of the Wilson coefficient is initialized on the fly using the python `lambda` built-in command. Any argument of the Wilson coefficients functions can be assigned a default value, in the example above \(r=1\) \(^3\). According to Table 1 the operators \(O_1\) and \(O_{M,0,0}\) are equivalent. This means that the Hamiltonian defined above can also be initialized setting:

```python
wc={('M',0,0): lambda M, r=1 : [(1.+r)/M**2, (1-r)/M**2] }.
```

The calculation of the differential WIMP-nucleus scattering rate of Eq. (A.3) requires a sodium-iodide target. In a realistic experiment like DAMA [19], COSINE [20] or ANAIS [21] sodium and iodine have different quenching factors that need to be taken into account in order to obtain the correct spectral shape. Notice, however, that the quenching is a property of both the target and a specific detector. This means that by defining sodium iodide as:

```python
nai_no_quenching=WD.Na+WD.I
```

the target will have no quenching attribute:

```python
['quenching' in dir(e) for e in nai_no_quenching.element]
[False, False]
```

because in such object the experimental information is missing. If, however, the directory `WimPyDD/Experiments/dama` contains files with quenching information (see Appendix C and Table 2) the command:

|  
|  
|---

\(^3\)The same variable can appear in more than one Wilson coefficient. Assigning it different default values in different Wilson coefficients may lead to unexpected results.
Dama = WD.experiment('dama')

dama = WD.experiment('dama')

creates an experiment object with a target attribute that now has quenching factors:

```python
dama = WD.experiment('dama')

na = dama.target
['quenching' in dir(e) for e in na.element]
[True, True]
```

So, as explained in Section 3.2, in order to calculate the differential rate as a function of the electron–equivalent energy one needs to use the target nai instead of nai_no_quenching in the diff_rate function, so that the argument energy is interpreted as $E_{ee}$. As far as the halo function stream contributions $\delta \eta_k^{(0)}$ are concerned they are calculated for a standard Maxwellian with standard parameters by:

```python
vmin, delta_eta0 = WD.streamed_halo_function()
```

(see Appendix E). By default 1000 values are tabulated, which is usually more than enough to accurately approximate the velocity integral. Finally, the differential rate is given by:

```python
er_vec = np.linspace(0.1, 20, 100)
mchi = 20.

diff_rate = [WD.diff_rate(nai, SI, mchi, er,
    vmin, delta_eta0, M=1e3) for er in er_vec]
import matplotlib.pyplot as pl
pl.plot(er_vec, diff_rate)
```

in terms of the model parameters $M$ and $r$ that are passed as a keyworded, variable-length argument list. If some parameters are not passed their default values are used if existing, otherwise they are fixed to 1. The last command uses Matplotlib to plot the output shown by thin solid red curve in Fig. 2. As already pointed out in this case the energy parameter is interpreted as the electron–equivalent energy $E_{ee} = q_T(E_R)E_R$ (see Appendix A), since both sodium and iodine have the quenching attribute.

The behaviour of every WimPyDD routine can be tuned by changing the default values of additional parameters that can be inspected issuing in a help command. For instance the argument elements_list allows to plot the separate contributions of sodium and iodine:

```python
na, i = na.element
diff_rate_na = [WD.diff_rate(nai, SI, mchi, er,
    vmin, delta_eta0, elements_list=[na], M=1e3)
    for er in er_vec]
diff_rate_i = [WD.diff_rate(nai, SI, mchi, er,
    vmin, delta_eta0, elements_list=[i], M=1e3)
    for er in er_vec]
```

Such contributions are shown in Fig. 2 by the blue dotted and green dashed lines, respectively.
Figure 2. Expected signals for the effective Hamiltonian of Eq.(3.1) with $m_\chi=20$ GeV and $r=1$ on sodium iodide. **Thin lines:** output of `diff_rate` for the differential rate $dR/dE_{ee}$ (Eq. (A.4)); **thick lines:** output of the `wimp_dd_rate` routine for the integrated rate $S_{E_1,E_2}$ (Eq. (2.19)) assuming binning and detector response of the DAMA experiment (the last bin is arbitrarily averaged over a wider range). **Solid lines:** NaI; **dotted lines:** contribution from scatterings off Na; **dashed line:** contribution from scattering off I.

### 3.5.2 Integrated rate with detector response

The `diff_rate` routine does not include the effects of experimental binning and of the detector response. In order to include such effects the `wimp_dd_rate` must be used, which requires to instantiate an experimental set up with the `experiment` class and to calculate the integrated response functions of Eq. (2.18). In particular, the following instructions:

```python
WD.load_response_functions(dama, SI, j_chi=0.5)
e,s0=WD.wimp_dd_rate(dama, SI, vmin, delta_eta0, mchi=20, M=1e3, r=1)
e,s0_na=WD.wimp_dd_rate(dama, SI, vmin, delta_eta0, mchi=20, elements_list=[na], M=1e3, r=1)
e,s0_i=WD.wimp_dd_rate(dama, SI, vmin, delta_eta0, mchi=20, elements_list=[i], M=1e3, r=1)
```

use the `dama` object instantiated in Sec. 3.5.1 to produce as an output the thick lines in Fig. 2 according to the information about the binning and the detector response stored in the WimPyDD/Experiments/dama/ folder. In the same directory the file `exposure.tab` contains an array with the exposures in each energy bin. In order to get the `wimp_dd_rate` output in events/kg/day/keV such array must contain the inverses of the bin widths $\delta_{E_1}$, $\delta_{E_2}$,...,$\delta_{E_n}$ i.e. must have the form $[1./\delta_{E_1}, 1./\delta_{E_2},...1./\delta_{E_n}]$ (see Appendix C.2).
On the other hand, the following instructions:

```python
def c9_tau(mchi, cross_section, r):
    hbarc2=0.389e-27
    mn=0.931
    mu=mchi*mn/(mchi+mn)
    cp=(np.pi*cross_section/(mu**2*hbarc2))**(1./2.)
    return cp*np.array([1.+r,1.-r])

c9=WD.eft_hamiltonian('c9',
    {9: c9_tau})
vmmin,delta_etal=WD.streamed_halo_function(
    yearly_modulation=True, n_vmin_bin=1000)
WD.load_response_functions(dama,c9)
e,s1=WD.wimp_dd_rate(dama, c9, vmin, delta_etal, 
cross_section=8.29e-33, mchi=9.3 , r=4.36)
```

use the same `dama` object to perform the following steps:

- define the function `c9_taul` that returns the two couplings (in GeV$^{-2}$) $c_9^\tau = (c_0^9, c_1^9)$ calculated in terms of the three parameters $m_\chi$, $r = c_0^9/c_1^9 = (c_0^9 - c_1^9)/(c_0^9 + c_1^9)$ and $\sigma_p = (c_0^9)^2 \mu_{\chi N}^2/\pi(hc)^2$ (in cm$^2$), i.e. 
  $c_0^9 = \sqrt{\pi \sigma_{ref}/(\mu_{\chi N}(hc)^2)}$, $c_1^9 = c_0^9 \times [1 + r, 1 - r]$;
• use the class `eff_hamiltonian` to define the model `c9` with effective Hamiltonian
  \[ \mathcal{H}_9 = \sum_{\tau=0,1} c_\tau^9 (m_\chi, \sigma_p, r) O_9(r) t^\tau, \]
  initializing the Wilson coefficients with the dictionary `{9:c9_tau};
• calculate the modulated halo function \( \delta \eta^j(v_k) \) of Eq. (2.11) using the `streamed_halo_function`
  routine with the argument `yearly_modulation=True` and saves the output in the two arrays `vmin, delta_eta1`;
• use the routine `load_response_functions` to calculate or load (if already present in the directory `WimPyDD/Experiments/dama`) the response functions of Eq. (2.18) for the `c9` effective model and a spin-1/2 WIMP (default value of spin);
• use the routine `wimp_dd_rate` to calculate the expected modulation amplitudes for the choice of parameters \( \sigma_p = 8.29 \times 10^{-33} \text{ cm}^2, m_\chi = 9.3 \text{ GeV}, r = 4.36 \) (such values correspond to the best fit of the DAMA/LIBRA-Phase2 experiment [19] for \( \mathcal{H}_9 \) from Ref. [4]). The `wimp_dd_rate` routine returns two arrays with the centers of the energy bins (in keV) and the corresponding predictions for the number of events. The energy bins are taken from the `data.tab` file in the `WimPyDD/Experiments/dama` directory.

The result is shown in Fig. 3 with the solid line and compared with the modulation amplitudes measured by DAMA/LIBRA-Phase2.

The same calculation can be easily extended to any combination of effective couplings by adding entries in the dictionary that parameterizes the Wilson coefficients. For instance, in Table II of Ref. [6] the effective model \( \mathcal{H} = \sum_{n=4,5,6} \sum_{\tau=0,1} c_n^\tau O_n(r) t^\tau \) is discussed in terms of the eight parameters \( m_\chi, \delta \) and \( c_0 = [c_4^0, c_4^1, c_5^0, c_5^1, c_6^0, c_6^1] \). The latter couplings vector is further expressed in terms of a direction \( \tilde{c}_0 = c_0 / |c_0| \) in the coupling space, and of an effective cross section parameterizing the couplings’ intensity, \( \sigma_{eff} = |c_0|^2 \mu^2_{\chi N} / \pi (\hbar c)^2 \). In particular for \( j_\chi = 1/2 \) the tension between the DAMA experiment and the constraints from other experiments is found to be minimized by: \( m_\chi = 11.64 \text{ GeV}, \delta = 23.74 \text{ keV}, c_0 = [-0.00139183, -0.00145925, -0.00318353, -0.01660634, 0.69199713, 0.72169939] \) and \( \sigma_{eff} = 4.68 \times 10^{-28} \text{ cm}^2 \). In WimPyDD such non–trivial effective model can be easily implemented with a few lines of code:

```python
def c_tau(mchi,sigma,c_tilde):
    hbarc2=0.389e-27
    mn=0.931
    mu=mchi*mn/(mchi+mn)
    c_abs=(mu**2*hbarc2/(np.pi*sigma))**(-0.5)
    return c_abs*c_tilde

wc={4: lambda mchi,s,c: c_tau(mchi,s,c)[0:2],
   5: lambda mchi,s,c: c_tau(mchi,s,c)[2:4],
   6: lambda mchi,s,c: c_tau(mchi,s,c)[4:6]}

c_456=WD.eft_hamiltonian('c_456',wc)

WD.load_response_functions(dama,c_456)
c_tilde=np.array([-0.00139183, -0.00145925, -0.00318353, -0.01660634, 0.69199713, 0.72169939])
```

- 18 -
mchi=11.64102564102564
delta=23.73913043478261
cross_section=4.684124873205523e-28
pl.plot(*WD.wimp_dd_rate(dama,c_456,vmin,delta_etal1,
mchi,delta=delta,s=cross_section,c=c_tilde))

Notice that in this case the model is inelastic (a \( \delta = m_{\chi'} - m_\chi \) parameter different from zero is used in Eq. (2.13) for the \( v_{\text{min}} \) parameter). Moreover, as already pointed out, in the Wilson coefficients the \texttt{mchi} and \texttt{delta} arguments are reserved and passed as positional arguments, while any other parameter can acquire an arbitrary name and is passed as a keyworded variable-length argument list. The corresponding result, plotted by the last instruction, is shown in Fig 3 by the solid red line and reproduces that of Fig 7 of [6]. Such prediction must be compared with the constraints from other experiments. For instance, by filling up the directory \texttt{WimPyDD/Experiments/xenon1t} with all the relevant information for the XENON1T experiment [22] (see Appendix C) one can calculate the corresponding number of events in the range 3 PE < \( S_1 < 70 \) PE with the following instructions:

\[
\text{xe=} \text{WD.target('Xe')}
\text{xenon1t=} \text{WD.experiment('xenon1t',xe)}
\text{WD.load_response_functions(xenon1t,c_456)}
\text{WD.wimp_dd_rate(xenon1t,c_456,vmin,delta_etal1,
mchi,delta=delta,s=cross_section,c=c_tilde)}
\text{(array([36.5]), array([4.78777365]))}
\]

In this case \texttt{wimp_dd_rate} returns the center of the only “bin”, as well as a total number of 4.78 events for an exposure of 362440 kg day (provided in the file \texttt{exposure.tab}). Such value is indeed consistent at 90% C.L. with the 7 candidate events measured in [22].

The evaluation of the binned signals in this Section requires a triple integration, over the WIMP velocity \( v \), the nuclear recoil energy \( E_R \) and the visible energy \( E' \). WimPyDD performs the double integral over \( E_R \) and \( E' \) only once and stores the response functions for later interpolation. Moreover the sums in Eqs (2.11) that substitute the velocity integral are optimized for speed in \texttt{numpy}. As a consequence the \texttt{wimp_dd_rate} routine is well suited for large iterations over the input parameters \texttt{par1,par2,...}.

### 3.5.3 Exclusion plot

A familiar way to show constraints from DD experiments is using exclusion plots in the mass–cross section plane. This requires sometimes sophisticated procedure of background subtraction and/or likelihood minimization. The \texttt{WimPyDD} code provides the simple routine \texttt{mchi_vs_exclusion} that allows to estimate the upper bound on any parameter \( \lambda \) that can be factorized from the rate by simply comparing the output of \texttt{wimp_dd_rate} with \( \lambda = 1 \) to the experimental upper bounds on the count rate in each energy bin (that the user can include in the \texttt{data.tab} experiment file) and taking the most stringent constraint. This is obtained by calling \texttt{mchi_vs_exclusion} without passing the \( \lambda \) argument (so that it is set to 1 by default) or passing \( \lambda = 1 \). For instance, in the case a standard isoscalar Spin–Independent interaction driven by the operator \( \mathcal{O}_1 \) the expected rate is proportional to the WIMP–proton cross section \( \sigma_p = (c_1^p)^2 \mu_{\chi N}^2 / \pi \) (equal to the WIMP–neutron cross section \( \sigma^n \)). To get the exclusion plot
Figure 4. XENON1T exclusion plot for a standard spin–independent interaction as a function of the WIMP mass $m_\chi$. **Left–hand plot:** upper bound on WIMP–proton cross section; **Right–hand plot:** upper bound on the effective scale $M$.

on $\sigma^p$ one must parameterize the coupling $c_1^p$ in terms of $\sigma^p$ and call `mchi_vs_exclusion` without fixing $\sigma^p$ (or setting it to unity):

```python
hbarc2=0.389e-27
mn=0.931
wc_SI={1: lambda mchi,sigma_p: np.sqrt(sigma_p*np.pi/hbarc2)*
(1./mn+1./mchi)*np.array([2.,0])}
SI=WD.eft_hamiltonian('SI',wc_SI)
mchi,sigma=WD.mchi_vs_exclusion(xenon1t, SI, vmin, delta_eta0)
pl.plot(mchi,sigma)
```

The output is shown in the left–hand plot of Fig. 4 with the red dashes, while the solid blue line is result of Ref. [22].

An appropriate reparameterization of the Wilson coefficients in `eft_hamiltonian` allows to use `mchi_vs_exclusion` to get exclusion plots on any parameter the expected rate is proportional to. For instance, the following few lines get the lower bound on the effective scale $M$ if the Wilson coefficient is parameterized as $c_1^p = 1/M^2$:

```python
SI_M=WD.eft_hamiltonian('SI_M',{1: lambda M: 1./M**2*np.array([2,0])})
mchi,one_over_M4=WD.mchi_vs_exclusion(xenon1t, SI_M, vmin, delta_eta0)
pl.plot(mchi,one_over_M4**(-1./4.))
```

In this case, since the expected rate is proportional to $M^{-4}$, an upper bound on the latter quantity is obtained if `mchi_vs_exclusion` is called without the $M$ argument (this is equivalent to passing $M=1$ since $M$ has no default value). The plot of the output in terms of $M = (M^{-4})^{-1/4}$ is shown in the right–hand plot of Fig. 4.
A Response functions

In this Section we derive explicitly Eq. (2.18) and the expressions of the integrated response functions discussed in Section 2.

The expected number of events in a WIMP DD experiment in the interval of visible energy $E_R'_{1} \leq E_R' \leq E_R'_{2}$ is:

$$ R[E_R'_{1},E_R'_{2}](t) = \sum_T \int_{E_R'_{1}}^{E_R'_{2}} dE_R' \left( \frac{dR}{dE_R'} \right)_T(t), \quad (A.1) $$

where $T$ indicates the target nuclei present in the detector. For a given target $T$:

$$ \left( \frac{dR}{dE_R'} \right)_T(t) = \int_{0}^{\infty} dE_R \left( \frac{dR}{dE_R} \right)_T(t) G[E', E_{ee}] \epsilon(E'). \quad (A.2) $$

In the equations above $E_R$ is the recoil energy deposited in the scattering process (indicated in keVnr), while $E_{ee}=q_T(E_R)E_R$ (indicated in keV) is the fraction of $E_R$ that goes into ionization and scintillation (with $q_T(E_R)$ the target quenching factor) and $G(E', E_{ee})$ is the effect of the energy resolution (so that $E_R'$ is measured instead of $E_{ee}$ through a calibration procedure$^4$). Finally $\epsilon(E')$ is the measured experimental acceptance. The differential rate is given by:

$$ \left( \frac{dR}{dE_R} \right)_T(t) = MN_T T_0 \int_{v_{T,\text{min}}(E_R)}^{v_{\text{esc}}(E_R)} \frac{\rho_\chi}{m_\chi} v \left( \frac{d\sigma}{dE_R} \right)_T(v) f(\vec{v}, t) d^3v, \quad (A.3) $$

with $f(\vec{v}, t)$ the WIMP velocity distribution in the Earth’s rest frame. In Eq. A.3 $N_T = N_A1000/m_N$ ($N_A=$Avogadro number) is the number of targets in one kg of detector, $M$ is the mass of the detector (so that $MN_T$ is the total number of targets $T$), $T_0$ the time of exposure, $\rho_\chi$ is the mass density of Dark Matter in the neighborhood of the Sun, $m_\chi$ the WIMP mass (so that $\rho_\chi/m_\chi$ represents the WIMP number density). In particular, using the piece–wise definition of (Eq. 2.5) in Eq. (A.3) one gets:

$$ \left( \frac{dR}{dE_R} \right)_T(t) = MN_T T_0 \int_{v_{T,\text{min}}(E_R)}^{v_{\text{esc}}(E_R)} \frac{\rho_\chi}{m_\chi} v \left[ \frac{d\sigma}{dE_R} (v) \right]_T \sum_k \lambda_k(t) \delta(v-v_k)dv, $$$$ = MN_T T_0 \sum_{v_k>v_{\text{min}}(E_R)}^{N_k} \frac{\rho_\chi}{m_\chi} v_k^2 \left[ \frac{d\sigma}{dE_R} (v_k) \right]_T \delta\eta_k(t) \Theta(v_k-v), \quad (A.4) $$

$^4$In the case of liquid scintillators such as XENON1T [22] the electron–equivalent energy is substituted by the average number $<\nu>$ of photo-electrons (PE), the visible energy is substituted by the observed number of PE $S_1$ and the light–yield $L$ takes the place of the quenching factor, with $S_1 = L <\nu>$. 

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Indicating with $j_T$ the target spin [10]:

\[
\left( \frac{d\sigma}{dE_R} \right)_T = \frac{2m_T c^2}{4\pi v^2} \left[ \frac{1}{2j_T + 1} \frac{1}{2j_T + 1} \sum_{\text{spin}} |M(q)|^2 \right],
\]

(A.5)

is the differential cross section in terms of the scattering amplitude averaged over the initial WIMP and target spins. In non–relativistic effective theory the latter is given by:

\[
\frac{1}{2j_T + 1} \sum_{\text{spin}} |M(q)|^2 = \frac{4\pi}{2j_T + 1} \sum_{\tau\tau'} \sum_l R_{\tau\tau'}^l (q, v) W_{l,T}^{\tau\tau'} (q).
\]

(A.6)

In the equation above the WIMP and nuclear physics are factorized in the two $R_{\tau\tau'}^l$ and $W_{l,T}^{\tau\tau'}$ functions, respectively, with $\tau, \tau' = 0, 1$ the nuclear isospin while $l = M, \Sigma', \Phi', \Phi' M, \Phi', \Delta, \Delta\Sigma'$ represent one of the possible nuclear interaction types, in the single–particle interaction limit [9, 10]. Moreover, in Eqs. (A.5) and (A.6) $q$ represents the transferred momentum:

\[
q = \sqrt{2m_T E_R}.
\]

(A.7)

Explicit expressions of the WIMP response functions $R_{\tau\tau'}^l$ are provided in [10] and [14] for the two sets of operators discussed in Appendix B. They can be decomposed as:

\[
R_{\tau\tau'}^l (q, v) = R_{0,0}^\tau (q) + R_{1,1}^\tau (q) (v^2 - v_{T,\min}^2),
\]

(A.8)

while power/exponential expansions of the nuclear response functions $W_{l,T}^{\tau\tau'}$ have been provided in [10] and [23] for most targets $T$ used in direct detection experiments. A direct substitution of Eqs. (A.2, A.3, A.5, A.6, A.8) in Eq. (A.1) yields:

\[
R_{[E'_1, E'_2]} (t) = \int dE_R \int dE' \int dE_R' \int dE_R \int d^3v f(\vec{v}, t) \frac{c^2}{v}
\]

\[
\times N_T M T_0 \frac{m_T}{2} G \left[ E', q_T (E_R) E_R \right] \epsilon (E')
\]

\[
\times \frac{4\pi}{2j_T + 1} \sum_{\tau\tau'} \sum_l \left\{ R_{0,0}^\tau (q) + R_{1,1}^\tau (q) (v^2 - v_{T,\min}^2) \right\} W_{l,T}^{\tau\tau'} (q).
\]

(A.9)

Introducing the speed velocity distribution:

\[
f(v, t) \equiv \int d\Omega_v f(\vec{v}, t), \quad v \equiv |\vec{v}|,
\]

(A.10)

the order of the two integrals in $E_R$ and $v$ can be inverted [16]. In particular:

\[
\int_0^\infty dE_R \int_{v_{T,\min}(E_R)}^\infty dv \int_{v_{T,\max}(E'_R)}^{E_{\max}(v)} dE_R \rightarrow \int v_{T,\max} dE' \int_{E_R^{\min}(v)}^{E_R^{\max}(v)} dE_R
\]

(A.11)

with $E_R^{\min,max}(v)$ and $v_{T,\max}$ given by Eqs. (2.14) and (2.2). In this way Eq. (A.9) can be recast in the form:

\[
R_{[E'_1, E'_2]} (t) = \int_{v_{T,\max}}^{\infty} dv H_{[E'_1, E'_2]} (v) f(v, t),
\]

(A.12)
with:

\[ \mathcal{H}_{[E_1', E_2']}^{(v)}(v) = \frac{\rho_\chi}{m_\chi} \frac{1}{\pi v} \sum_T \int_{E_{R,\text{min}}^{(v)}}^{E_{R,\text{max}}^{(v)}} dE_R \left\{ \mathcal{R}_T^0(E_R) + \mathcal{R}_T^1(E_R) \left( v^2 - v_{T,\text{min}}^2(E_R) \right) \right\} \tag{A.13} \]

\[ \mathcal{R}_T^i(E_R) = \int_{E_i'}^{E_2'} dE' r_T^i(E_R, E'), \quad i = 0, 1, \tag{A.14} \]

and:

\[ r_T^i(E_R, E') = M T_0 N_T \frac{m_T}{2} \epsilon(E') G (E', q_T(E_R) E_R) \frac{4\pi}{2J_T + 1} \sum_{\tau' T} \sum_l \mathcal{R}_{\tau' T}^{i}(q) W_{\tau' T}(q). \tag{A.15} \]

The speed distribution \( f(v) \) can be written as [16]:

\[ f(v, t) \equiv -v \frac{d}{dv} \eta(v, t), \tag{A.16} \]

so that integrating by parts one gets Eq. (2.1) where:

\[ \mathcal{R}_{[E_1', E_2']}^{(v)}(v) = \frac{d}{dv} \left[ v \mathcal{H}_{[E_1', E_2']}^{(v)}(v) \right], \tag{A.17} \]

Substituting Eq. (2.5) in Eq. (2.1), with \( \mathcal{R} \) and \( \mathcal{H} \) given by Eqs. (A.17,A.13) one gets:

\[ R_{[E_1', E_2']}^{(v)}(v, t) = \sum_T \rho_\chi \frac{1}{m_\chi} \int_{v_{\text{min}}}^{v_{\text{max}}} dv' \frac{d}{dv'} \left\{ \frac{c^2}{v} \int_{E_{R,\text{min}}^{(v')}}^{E_{R,\text{max}}^{(v')}} dE_R \left\{ \mathcal{R}_T^0(E_R) + \mathcal{R}_T^1(E_R) \left( v'^2 - v_{T,\text{min}}^2(E_R) \right) \right\} \right\} \times \sum_{k=1}^{N_T} \delta \eta_k(t) \theta(v_k - v) = \]

\[ \sum_T \rho_\chi \frac{1}{m_\chi} \sum_{k=1}^{N_T} \delta \eta_k(t) \times \int_{E_{R,\text{min}}^{(v_k)}}^{E_{R,\text{max}}^{(v_k)}} dE_R \left\{ \mathcal{R}_T^0(E_R) + \mathcal{R}_T^1(E_R) \left( v_k^2 - v_{T,\text{min}}^2(E_R) \right) \right\}, \tag{A.18} \]

which is equivalent to Eq. (2.12).

B Sets of non–relativistic effective operators

WimPyDD allows to use two alternative sets of non–relativistic effective operators for the Hamiltonian of Eq. (2.15): the set introduced in Ref. [9, 10] for a WIMP spin \( j_\chi \leq 1/2 \) and the set of Ref. [14], valid for any value of \( j_\chi \).

In Refs. [9, 10] the operators \( \mathcal{O}_j \) have been indicated with progressive numbers from 1 to 16. However \( \mathcal{O}_2 \) is neglected because it is quadratic in the WIMP incoming velocity while \( \mathcal{O}_{16} \) can be written as a linear combination of \( \mathcal{O}_{12} \) and \( \mathcal{O}_{15} \). WimPyDD allows to use any of the remaining 14 independent operators by setting the keys of the \( \text{wc} \) dictionary to one of the integers 1,3,4,...,15.
Table 1. Non-relativistic Galilean invariant operators $\mathcal{O}_j$ introduced in [10–12]) for a dark matter particle of spin 0, 1/2 and 1, and their relation with the WIMP–nucleon operators $\mathcal{O}_{X,s,l}$ defined in Ref. [14].

| $\mathcal{O}_j$ | $\mathcal{O}_{X,s,l}$ | $\mathcal{O}_{M,0,0}$ | $\mathcal{O}_{\Phi,0,1}$ |
|------------------|----------------------|------------------|------------------|
| $\mathcal{O}_1$  | 1                    | $\mathcal{O}_{M,0,0}$ | $\mathcal{O}_{\Phi,0,1}$ |
| $\mathcal{O}_2$  | $(\vec{p}_N^+)^2$   | N.A.              |                  |
| $\mathcal{O}_3$  | $-i\vec{S}_N \cdot (\vec{q} \times \vec{v}_N^+)$ | $\mathcal{O}_{\Phi,0,1}$ |                  |
| $\mathcal{O}_4$  | $\vec{S}_N \cdot \vec{S}_N$ | $\mathcal{O}_{\Sigma,1,0}$ |                  |
| $\mathcal{O}_5$  | $-i\vec{S}_N \cdot (\vec{q} \times \vec{v}_N^+)$ | $\mathcal{O}_{\Delta,1,1}$ |                  |
| $\mathcal{O}_6$  | $(\vec{S}_N \times \vec{q})(\vec{S}_N \times \vec{q})$ | $\mathcal{O}_{\Sigma,1,2}$ |                  |
| $\mathcal{O}_7$  | $\vec{S}_N \times \vec{v}_N^+$ | $\mathcal{O}_{0,0}$ |                  |
| $\mathcal{O}_8$  | $\vec{S}_N \times \vec{v}_N^+$ | $\mathcal{O}_{1,0}$ |                  |
| $\mathcal{O}_9$  | $-i\vec{S}_N \cdot (\vec{S}_N \times \vec{q})$ | $\mathcal{O}_{1,1}$ |                  |
| $\mathcal{O}_{10}$ | $-i\vec{S}_N \times \vec{q}$ | $\mathcal{O}_{0,1}$ |                  |
| $\mathcal{O}_{11}$ | $-i\vec{S}_N \times \vec{q}$ | $\mathcal{O}_{M,1,1}$ |                  |
| $\mathcal{O}_{12}$ | $\vec{S}_N \cdot (\vec{S}_N \times \vec{v}_N^+)$ | $\mathcal{O}_{-\Phi,1,0}$ |                  |
| $\mathcal{O}_{13}$ | $\mathcal{O}_{10}\mathcal{O}_8$ | $-\mathcal{O}_{\Phi,1,1}$ |                  |
| $\mathcal{O}_{14}$ | $\mathcal{O}_{11}\mathcal{O}_7$ | $-\mathcal{O}_{\Omega,1,1}$ |                  |
| $\mathcal{O}_{15}$ | $-\mathcal{O}_{11}\mathcal{O}_3$ | $-\mathcal{O}_{\Phi,1,2}$ |                  |
| $\mathcal{O}_{16}$ | $-\mathcal{O}_{10}\mathcal{O}_5$ | $-\mathcal{O}_{\Phi,1,2} - \vec{q}^2 \mathcal{O}_{\Phi,1,0}$ |                  |
| $\mathcal{O}_{17}$ | $-\vec{q} \cdot \mathcal{S}_N \cdot \vec{v}_N^+$ | $\mathcal{O}_{\Delta,2,1}$ |                  |
| $\mathcal{O}_{18}$ | $-\vec{q} \cdot \mathcal{S}_N \cdot \vec{S}_N^+$ | $\mathcal{O}_{\Sigma,2,1} - \frac{1}{2} \mathcal{O}_{\Sigma,0,1}$ |                  |
| $\mathcal{O}_{19}$ | $\vec{v}_N \cdot \mathcal{S}_N \cdot \vec{v}_N^+$ | $\mathcal{O}_{M,2,2} + \frac{1}{2} \vec{q}^2 \mathcal{O}_{M,0,0}$ |                  |
| $\mathcal{O}_{20}$ | $\left(\vec{S}_N \times \vec{q}\right) \cdot \mathcal{S}_N \cdot \vec{q}$ | $\mathcal{O}_{\Sigma,2,2}$ |                  |
| $\mathcal{O}_{21}$ | $\vec{v}_N \cdot \mathcal{S}_N \cdot \vec{v}_N^+$ | $\mathcal{O}_{\Delta,2,1}$ |                  |
| $\mathcal{O}_{22}$ | $-\left(\vec{q} \times \vec{v}_N^+\right) \cdot \mathcal{S}_N \cdot \vec{S}_N$ | $\mathcal{O}_{\Phi,2,1} - \frac{1}{2} \mathcal{O}_{\Phi,0,1}$ |                  |
| $\mathcal{O}_{23}$ | $-\vec{q} \cdot \mathcal{S}_N \left(\vec{S}_N \times \vec{v}_N^+\right)$ | $\mathcal{O}_{\Phi,2,1} + \frac{1}{2} \mathcal{O}_{\Phi,0,1}$ |                  |
| $\mathcal{O}_{24}$ | $-\vec{v}_N \cdot \mathcal{S}_N \left(\vec{S}_N \times \vec{q}\right)$ | $\mathcal{O}_{\Phi,2,1} - \frac{1}{2} \mathcal{O}_{\Phi,0,1}$ |                  |

In Ref. [14] such base has been extended by the set of irreducible operators $\mathcal{O}_{X,s,l}$ classified in terms of the 5 basic nuclear currents $X = M, \Omega, \Sigma, \Delta, \Phi$, of the operator rank $s = 0, 1, \ldots, 2j_X$ and of the parameter $l$, related to the explicit power of the transferred momentum $q$ appearing in the operator (possible values of $l$ are: $l = s$ for $X = M, \Omega; l = s-1, s, s+1$ for $X = \Sigma, \Phi; l = s-1, s$ for $X = \Delta$). See [14] for the explicit definitions of the $\mathcal{O}_{X,s,l}$ operators. For $j_X \leq 1$ the relation between the set of Ref. [14] and that of Refs. [9, 10] (including there extension to some spin-1 operators [11, 12]) is listed in Table 1.

As a consequence, besides an integer, each key $n$ of the dictionary wc can also be a tuple $(X, s, l)$ with $X$ a string among 'M', 'Omega', 'Sigma', 'Delta' and 'Phi' and $s, l$ two integers following the restrictions explained above.

C Initializing the experiment directory

The calculation of the integrated functions of Eq. (2.18), which include the effect of the detector’s response, require to fix the target $T$, the energy intervals $[E_1, E_2]$, as well as the differential response functions $r_T(E_R, E')$ of Eq. (A.15). The latter depend on the exposure $MT_0$, the efficiency $\epsilon(E')$, the energy resolution $\mathcal{G}(E', E_{ee})$ and the quenching factors $q_T(E_R)$ (for each element in the target). As explained in Section 3.3.4 at instantiation the

\footnote{WimPyDD does not allow to mix the two different sets of operators in the same Hamiltonian.}
Table 2. Files in the experiment subfolder containing the information to calculate the response functions.

| Physical quantity(unit) | Default(if missing file) | File name                        |
|-------------------------|--------------------------|----------------------------------|
| Target material         | no default               | target.tab                       |
| $MT_0$(kg day)          | 1                        | exposure.tab                     |
| $\epsilon(E')$         | 1                        | efficiency.tab or efficiency.py  |
| $G(E',E_{ee})$          | $\delta(E' - E_{ee})$    | resolution.py                    |
| $q_T(E_R)$              | 1                        | <element_name>_quenching.py or <element_name>_quenching.tab (ex: xenon_quenching.tab) |
| $[E_1',E_2']$(keV)      | $E_1'=E_2'=1$ keV        | data.tab                         |
| Modifier (see Appendix C.6) | 1                        | modifier.tab                     |

The `experiment` class stores each of these elements in an appropriate attribute, reading the information relevant to each of them from a separate file contained in a sub-folder of the WimPyDD/Experiments folder of the working directory. The name of the subfolder is passed as an argument to the `experiment` class. The list of files is given in Table 2. For all of them if the file is missing the default value indicated in the Table is adopted. In particular the target material has no default and can be either passed as a `target` object (see 3.3.1) to the `experiment` class, or provided in the file `target.tab` as a valid input string for the `target` class.

All input files must contain plain text. In the following we review each of them. All the lines of a `.tab` file that do not match the expected format are ignored with the exception of the first, that is interpreted as a help string. The `.py` files are loaded as ordinary libraries, and must contain a valid python function implementing the relevant quantity (energy resolution, efficiency, quenching). Such function can have an arbitrary name (WimPyDD loads the first function defined in the file) and its user-provided help (within `'...''` triple quotation marks) is loaded as a help string. All help strings are printed issuing a `print` command of the `experiment` object. A few examples of experiment directories are provided with the WimPyDD distribution.

C.1 Target file

If present the target file must contain a string with a valid input for the WD.target class, for instance Ge, CF3I or NaI (no quotation marks). If the target.tab file is not provided a target object should be passed as a parameter to the experiment class. In this case the corresponding target.tab file will be added to the experiment directory. WimPyDD will prompt the user for an input if neither a target object is passed to the experiment class nor a target.tab is provided. Moreover it will produce a warning if the user passes a target
object to the `experiment` class that does not match the content of an existing `target.tab` file in the experiment directory.

C.2 Exposure file

This file can contain either a float with the exposure $MT_0$ in kg/day or a list/array with a different exposure for each of the experimental bins contained in `data.tab`, and controls the output of the `wimp_dd_rate` routine. Setting the content of `exposure.tab` to 1 (or, equivalently, if the `exposure.tab` file is missing) will produce an output normalized to events/kg/day. Moreover an output in events/kg/day/keV will be obtained by providing in `exposure.tab` a list or array with the inverses of the energy bin widths contained in `data.tab`.

C.3 Efficiency and quenching files

These files must contain either two columns with a sampling of the arguments and values of the function to be used for interpolation (a simple linear interpolation is used) or a valid Python function. Notice that the efficiency function $\epsilon$ must depend on the visible energy $E'$ (in keV) while the quenching (or light yield) $Q(E_R)$ must depend on the recoil energy $E_R$ (also in keV). A different file for the quenching factor of each element in the target can be provided, with the naming convention of Table 2.

C.4 Energy resolution file

Since the function $G(E', E_{ee})$ takes two arguments only a `.py` file can be provided with a regular Python function in the two variable $E'$ (visible energy) and $E_{ee}$ (electron-equivalent energy) in keV:

```python
def resolution(e_prime,e_ee):
    ...
```

C.5 Data file

The file `data.tab` must contain the energy bins $[E'_1, E'_2]$ needed for the calculation of the response function of Eq. (2.18) that affects the output of the `wimp_dd_rate` routine. Each line of the `data.tab` file corresponds to a different energy bin and can be in different format, as summarized in Table 3. In particular, if a line contain a single float `wimp_dd_rate` will return the differential rate at the corresponding value of the energy and the response functions of Eq. (2.18) will not be integrated upon $E'$ (the differential rate can be calculated more efficiently using the `diff_rate` routine, although without the effect of the detector’s response). On the other hand two floats will be interpreted as an interval of visible energy $E'$. If present, the information following the two floats of an energy bin is used by `mchi_vs_exclusion` to calculate a 90% C.L. upper bound: in this case a single integer will be interpreted as a measured number of counts with Poissonian fluctuation, two floats as a number of counts with the corresponding Gaussian error. Each line of the `data.tab` file can have different format (single energy value/energy interval, with/without upper bound information). Bins without upper bound information are neglected by the `mchi_vs_exclusion` routine.
Table 3. Accepted format of each line of the `data.tab` file.

| Line content | WimPyDD interpretation |
|--------------|-------------------------|
| 10           | $E'=10$ keV             |
| 10 20        | $[E'_1, E'_2]=[10,20]$ keV |
| 10 20 1      | $[E'_1, E'_2]=[10,20]$ keV, $N_{counts}=1$ events |
| 10 20 3.2 0.4| $[E'_1, E'_2]=[10,20]$ keV, $N_{counts}=3.2\pm0.4$ events |

C.6 Modifier

If present, the file `modifier.py` must contain a function

```python
f(er, eprime, exp, n_element, n_isotope, n_bin)
```

with $er=E_R$, $eprime=E'$, `exp` an object belonging to the `experiment` class, `n_element` and `n_isotope` two integers that specify the element in the `exp.target.element` array and the isotope, respectively and `n_bin` an integer identifying the energy bin (among those defined in `data.tab`). The default for the function is unity. At the time of calculating the integrated response functions $\bar{R}_{T,[E'_1, E'_2]}^{\text{int}}(E_R)$ the differential response functions $[\bar{r}_{T}^{\text{int}}(E_R, E')]_{jk}$ are multiplied times the modifier. Its purpose is to implement specific cases where the expected rate is not in the form of Eqs. (A.1,A.3), allowing, in principle, a different modifier for each target or energy bin. For instance, droplet detectors and bubble chambers such as COUPP [24], PICO60 [25] or PICASSO [26] are threshold detectors (i.e. a signal is detected only above some value of the deposited energy, which is fixed by changing the running parameters such as the temperature or the pressure). In this case the expected number of events is given by:

$$R = N_TM_T \int_0^{\infty} P(E_R) \frac{dR}{dE_R} dE_R,$$

where $P(E_R)$ is the probability that the energy $E_R$ will produce a signal if the energy threshold is fixed to $E_{th}$. The response function for such class of detectors requires that no energy resolution is provided while the $P(E_R)$ function is implemented through the file `modifier.py`.

D Adding new nuclear targets

Element targets are instantiated by the `element` class, that takes as an argument a string with the element symbol. By convention element symbols must begin with a capital letter. The string must correspond to a file in the directory `WimPyDD/Targets` containing the required information. For instance the xenon element, with symbol Xe, is instantiated with:

```python
xenon=WD.element('Xe')
```
and the class requires the text file "Xe.tab" in WimPyDD/Targets. The content of such file is the following:

|           |         |       |       |        |
|-----------|---------|-------|-------|--------|
| xenon     | xe      | 54    | 128   | 0.01910|
| 129       | 0.26401 | 0.5   | 12    |        |
| 130       | 0.04071 | 0     | 13    |        |
| 131       | 0.21232 | 1.5   | 14    |        |
| 132       | 0.26909 | 0     | 15    |        |
| 134       | 0.10436 | 0     | 16    |        |
| 136       | 0.08857 | 0     | 17    |        |

The first three lines contain the element full name, symbol, and atomic number Z. For each of the element isotopes each of the following lines initializes the atomic mass number A in the first column, the fractional abundance in the second column and the spin j_T in the third column. Finally the last column contains the internal integer code itar=1,..., 30 which is used to initialize the nuclear response functions W_{l,T}(q) provided in Refs. [10, 23] for the 30 isotopes T=^{12}C, ^{19}F, ^{23}Na, ^{28}Si, ^{70}Ge, ^{72}Ge, ^{73}Ge, ^{74}Ge, ^{76}Ge, ^{127}I, ^{128}Xe, ^{129}Xe, ^{130}Xe, ^{131}Xe, ^{132}Xe, ^{134}Xe, ^{136}Xe, ^{16}O, ^{40}Ar, ^{40}Ca, H, ^{3}He, ^{4}He, ^{14}N, ^{20}Ne, ^{24}Mg, ^{27}Al, ^{32}S, ^{56}Fe, ^{59}Ni. In particular, the following parameterization is used [10]:

\[ W_{l,T}^{\tau,\tau'}(q)e^{-2y}\sum_{n}a_{n}^{\tau,\tau'}y^{n}, \]  

where \( y = (qb/2)^2 \), \( b = \sqrt{41.467/(45A^{-1/3} - 25A^{-2/3})} \). The \( a_{n}^{\tau,\tau'} \) coefficients are contained at the line 8(itar - 1) + l + \tau + \tau' of the file

WimPyDD/Targets/Nuclear_response_functions/ 
nuclear_response_functions_coefficients_table.dat

where \( l = 1,...,8 \) corresponds to the 8 nuclear response functions \( M, \Sigma'', \Sigma', \Phi'', \Phi', \Delta, \Phi''M, \Delta\Sigma' \). Upon instantiation the element object acquires the method func_w, an array that contains a function of the single argument q for each isotope of the element. Such function returns an array with shape (8,2,2)=(l,\tau,\tau') with the values of the nuclear response functions of Eq. (D.1).

For new elements or isotopes for which numerical calculations of the \( W_{l,T}^{\tau,\tau'}(q) \) functions are not available the internal code itar must be set to zero. It is possible to provide the corresponding nuclear response function (or to override the default definitions of [10, 23]) adding the file <isotope_name>_func_w.py in the directory

WimPyDD/Targets/Nuclear_response_functions/ with <isotope_name> the isotope name, that must match one of the entries of the isotopes attribute of the element class. Such file must contain a custom definition of the nuclear response function with the same behaviour of the default one, i.e. it must depend on the single argument q and return an array with shape (8,2,2). For instance, in order to change \( W_{l,T} \) for \( T=^{129}Xe \) the custom definition must be contained in the file 129Xe_func_w.py with '129Xe' one of the entries of
the xenon isotopes array (a few examples of custom definition files are provided with the WimPyDD distribution). If itar=0 and no file is present the corresponding nuclear response functions are set to zero.

### E The halo function

WimPyDD contains a routine `streamed_halo_function` that calculates the $v_k$, $\delta\eta_k^{(0,1)}$ quantities needed by the `diff_rate` and `wimp_dd_rate`. The simple call:

```python
vmin, delta_eta0=Wstreamed_halo_function()
```

samples linearly the $\delta\eta_k^{(0)}$’s for a Maxwellian velocity distribution cut at the escape velocity in the Earth’s rest frame:

$$f(\vec{v},t) = N \left( \frac{3}{2\pi v_{\text{rms}}^2} \right)^{3/2} e^{-\frac{3\left(|\vec{v}+\vec{v}_{E,Gal}|\right)^2}{2v_{\text{rms}}^2}} \Theta(v_{\text{esc,Gal}} - |\vec{v} + \vec{v}_{E,Gal}(t)|), \quad (E.1)$$

$$N = \left[ \frac{\text{erf}(z) - 2\sqrt{\pi}e^{-z^2}}{z^2} \right]^{-1}, \quad (E.2)$$

with $v_{\text{esc,Gal}}$ the escape velocity in the Galactic rest frame and $z^2 = \frac{3v_{\text{esc,Gal}}^2}{2v_{\text{rms}}^2}$. By default hydrothermal equilibrium between the WIMP gas pressure and gravity is assumed, $v_{\text{rms}} = \sqrt{3/2|\vec{v}_{\text{rot,Gal}}|}$ with $\vec{v}_{\text{rot,Gal}}$ the galactic rotational velocity (such value can be modified using the argument `vrmss`). Moreover $\vec{v}_{E,Gal} = \vec{v}_{\text{rot,Gal}} + \vec{v}_{\text{Sun,rot}} + \vec{v}_{E,Sun}$, with $\vec{v}_{\text{Sun,rot}}$ the peculiar velocity of the solar system with respect to the Galactic rotational curve and $\vec{v}_{E,Sun}$ the velocity of the Earth around the Sun. The routine assumes the default values $v_{\text{esc,Gal}} = 550$ km/s, $\vec{v}_{\text{rot,Gal}} = (0, 220, 0)$ km/s, $\vec{v}_{\text{Sun,rot}} = (9, 12, 7)$ km/s (in the Galactic reference frame where the $z$ axis is in the direction perpendicular to the galactic plane, the $x$ axis points toward the galactic center and the velocity of the solar system points in the $y$ direction). Such values can be changed by using the arguments `v_esc_gal`, `v_rot_gal` and `v_sun_rot`, respectively. For $\vec{v}_{E,Sun}$ the expression in [18] is used. To calculate $\delta\eta_k^{(1)}$ the argument `yearly_modulation=True` must be used, and to get $\eta_k^{(0,1)}$ instead of $\delta\eta_k^{(0,1)}$ use `delta_eta=False`.

The routine can also be used for a user–defined velocity distribution. This requires to pass the argument `velocity_distribution_gal`. For instance, setting:

```python
def func(u,sigma_x,sigma_y,sigma_z):
    return np.exp(-0.5*(u[0]**2/sigma_x**2 + u[1]**2/sigma_y**2 + u[2]**2/sigma_z**2))
```

the corresponding time-averaged $\delta\eta_k^{(0)}$’s can be calculated by:

```python
vmin, delta_eta_0=Wstreamed_halo_function(
    velocity_distribution_gal=func,
    sigma_x=120, sigma_y=150, sigma_z=170)
```
Table 4. List of the main components of the WimPyDD code.

| Section | Equation | WimPyDD |
|---------|----------|---------|
| A       | \( \frac{d\sigma}{dE_R} T \) | (A.5) dsigma_der |
| A       | \( \frac{1}{2j_r+1} \frac{1}{2j_T+1} \sum_{\text{spin}} |\mathcal{M}(q)|^2 \) | (A.6) eft_amplitude_squared |
| A       | \( W_{T,T'}^{f,f} \) | (A.6) target.element[i].func_w |
| A       | \( \delta \eta_k \) | (2.5) streamed_halo_function |
| A       | \( \frac{dR}{dE_R} T \) | (A.4) diff_rate |
| A       | \( S_{[E_1,E_2]}^{0,1} \) | (2.7) and (2.8) wimp_dd_rate |
| 2       | \( \mathcal{H} = \sum_{\tau=0,1} \sum_j c_j^\tau \mathcal{O}_j |j^\tau \) | (2.15) eft_hamiltonian |
| 2       | \( \left[ \mathcal{R}_{T,[E_1^2,E_2^2]}^{a,a'} |(E_R)|_{j_k}^{\tau\tau'} \right] \) | (2.16) experiment.response_functions |

The user–define velocity distribution \texttt{func} must be a function of a three–dimensional array containing the WIMP velocity in the galactic rest frame. The parameters of \texttt{func} are passed with the keyworded variable-length argument list \texttt{**args} (the argument \texttt{v_rms} for the Maxwellian distribution is just a particular case of this). All the other parameters of the routine work in the same way as for a Maxwellian.

Both for a Maxwellian and for a user–defined velocity distribution the full expressions of Eqs. (2.9) and (2.10) (discretized as sums over the days of the year) can be used by setting \texttt{full_year_sample=True}. This can be time consuming, so that by default \texttt{full_year_sample = False}. In this case \( \eta(0) \) is approximated by setting \( \vec{v}_{E,Sun} \rightarrow 0 \). As far as the modulated component \( \eta(1) \) is concerned, in the Maxwellian case it is approximated by using a linear expansion in the parameter \( |\vec{v}_{E,Sun}|/|\vec{v}_{E,Gal}| \), while for the case of a user–defined velocity distribution it is calculated using the expression \( \eta(t = t_0) - \eta(t = t_0 + T/2) \) /2. Also \( t_0 \) can be changed by using the argument \texttt{modulation_phase} in days. Finally, \texttt{day_of_the_year} allows to calculate the halo function on a specific day of the year.

In the case when \texttt{velocity_distribution_gal} is used and the routine calculates numerical integrals the output is saved in the folder \texttt{Halo_functions} for later use to speed-up successive evaluations of the same halo function, unless \texttt{recalculate=True}.

F Summary of WimPyDD components

In table 4 we provide a short summary of the main components of the WimPyDD code with their correspondence to the Equations in Section 2 and Appendix A. To learn more about each of them use the Python help function.

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