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Calculating fusion neutron energy spectra from arbitrary reactant distributions

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Abstract

The Directional Relativistic Spectrum Simulator (DRESS) code can perform Monte-Carlo calculations of reaction product spectra from arbitrary reactant distributions, using fully relativistic kinematics. The code is set up to calculate energy spectra from neutrons and alpha particles produced in the D(d,n)^{3}He and T(d,n)^{4}He fusion reactions, but any two-body reaction can be simulated by including the corresponding cross section. The code has been thoroughly tested. The kinematics calculations have been benchmarked against the kinematics module of the ROOT Data Analysis Framework. Calculated neutron energy spectra have been validated against tabulated fusion reactivities and against an exact analytical expression for the thermonuclear fusion neutron spectrum, with good agreement. The DRESS code will be used as the core of a detailed synthetic diagnostic framework for neutron measurements at the JET and MAST tokamaks.

Keywords: nuclear reactions, relativistic kinematics, nuclear fusion, neutron spectrometry
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1. Introduction

In the interpretation and simulation of nuclear fusion experiments it is frequently of interest to calculate the energy spectrum of particles produced in various nuclear reactions occurring in the fusion plasma. The energy of a reaction product depends on the masses of the particles involved in the

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reaction and on the velocities of the reactants. Several different types of non-trivial velocity distributions occur in the magnetic and inertial confinement fusion experiments of today, which significantly affect the shape of the energy spectra of the particles produced in the fusion reactions. This is readily seen from measurements of neutron spectra from the D(d,n)^{3}He (DD) and T(d,n)^{4}He (DT) fusion reactions [1, 2, 3]. In these cases it is necessary to integrate over the reactant distributions and the reaction cross section in order to calculate the expected product spectrum.

This paper describes the Directional Relativistic Spectrum Simulator (DRESS) code, which calculates product spectra from two-body reactions between reactants with arbitrary velocity distributions. The input to the code is the masses of all particles involved in the reaction, the reactant distributions and the emission direction of the product particle under consideration. The calculations are performed by means of a Monte-Carlo simulation, using fully relativistic kinematics. The DRESS code has been developed primarily for the calculation of neutron and charged particle spectra from the DD and DT fusion reactions. However, any other two-body reaction can be simulated as well, by changing the cross section and the relevant masses used in the code.

The problem of calculating fusion product spectra has previously been addressed analytically in [4, 5], for the case of Maxwellian reactant distributions. A general method for deriving the product spectrum for arbitrary distributions, using classical kinematics, is presented in [6], with applications to a selection of special cases, such as a bi-Maxwellian, a beam distribution and an imploding shell.

In addition to the analytical work, there are also several references reporting the results of Monte-Carlo calculations of product spectra [7, 8, 9]. The main difference between these calculations and the DRESS code lies in the solution to the kinematics equation, to obtain the product energy. In the DRESS code a closed form expression for the energy is used, which gives the energy directly in the reference frame of interest. This is a different approach than the traditional method of evaluating the energy in the center of momentum (COM) reference frame and transforming the result back to the original frame. Furthermore, in addition to the calculated product spectrum, the DRESS code also returns an estimate of the Monte-Carlo uncertainty. This information is crucial in order to assess the reliability of the result, but it is not available from any of the earlier codes. Finally, in the references describing these codes fairly little information is given about the

details of the calculations, making it difficult for new users to understand how the codes work and what their range of applicability is. One aim of this paper is therefore to provide a detailed description of all the steps required to perform Monte-Carlo calculations of fusion product spectra.

The paper is organized as follows. The steps carried out during the Monte-Carlo calculations are presented in section 2. Section 3 presents the tests that have been performed in order to validate the DRESS code. Some examples illustrating the capabilities of the code are given in section 4. Finally, the main points of the paper are summarized in section 5, which also contains an outlook about potential applications of the code.

2. Calculations

A reaction of the form $a + b \rightarrow \alpha + \beta$ is considered, where the reactants a and b can have arbitrary velocity distributions $f_a(\mathbf{v}_a)$ and $f_b(\mathbf{v}_b)$. The purpose of the calculations is to find the energy spectrum of the product species α, emitted along a given unit vector $\mathbf{u}$. This is done by a Monte-Carlo simulation that proceeds through the following sequence of steps:

1. Randomly sample reactant velocities, $\mathbf{v}_a$ and $\mathbf{v}_b$, from their respective distributions, along with the corresponding statistical weights, w_a and w_b.
2. Calculate the energy of the product α, E_α, when this particle is emitted in direction $\mathbf{u}$.
3. Calculate the differential cross section, $\mathrm{d}\sigma/\mathrm{d}\Omega$, for the reaction under consideration, in order to compute the reaction rate.
4. Repeat the steps above to collect statistics. The product spectrum is obtained by collecting the Monte-Carlo events in a histogram with the appropriate weights.

Step 1 is straightforward, relying on nothing more than standard techniques involving pseudo-random numbers. Steps 2, 3 and 4 are described in more detail in the following sections.

2.1. Solve the kinematic equation

Throughout this paper, capital P is used to denote a momentum four-vector with total energy E and three momentum $\mathbf{p}$, i.e. $P = (E, \mathbf{p})$. The product of two four vectors, $P_a P_b = E_a E_b - \mathbf{p}_a \cdot \mathbf{p}_b$, is a scalar invariant, independent of the reference frame in which the product is evaluated. In

particular, the square of the four momentum for a particle a is simply the mass squared of that particle, $P_a^2 = m_a^2$. All equations are written in units in which the speed of light c is equal to 1.

For the two-body reaction considered here, four momentum conservation dictates that

$$P_{\rm tot} \equiv P_a + P_b = P_\alpha + P_\beta. \tag{1}$$

Rearranging and squaring this equation gives

$$P_{\rm tot} P_\alpha = \frac{s + m_\alpha^2 - m_\beta^2}{2}, \tag{2}$$

where $s = P_{\rm tot}^2$ is the first Mandelstam invariant and m_j is the mass of particle j. If particle α is emitted in the direction specified by $\mathbf{u} \equiv \mathbf{p}_\alpha / p_\alpha$, equation (2) becomes

$$E_{\rm tot} E_\alpha - \mathbf{p}_{\rm tot} \cdot \mathbf{u} p_\alpha = \frac{s + m_\alpha^2 - m_\beta^2}{2}. \tag{3}$$

Substituting $p_\alpha = (E_\alpha^2 - m_\alpha^2)^{1/2}$ gives an equation for E_α that can be put in the form of a quadratic equation, with solution

$$E_\alpha = \frac{A \pm \sqrt{A^2 - (1 - B^2)\left(A^2 + m_\alpha^2 B^2\right)}}{1 - B^2}, \tag{4}$$

where

$$\begin{aligned} A &= \frac{s + m_\alpha^2 - m_\beta^2}{2E_{\rm tot}}, \\ B &= \frac{\mathbf{p}_{\rm tot}}{E_{\rm tot}} \cdot \mathbf{u}. \end{aligned}$$

Equation (4) gives the energy of one of the particles produced in a two-body reaction, when the particle is emitted in the direction of the unit vector u. A solution of this form was previously used in the kinematics code described in [10]. Depending on the value of $P_{\rm tot}$, this equation can have 0, 1 or 2 physically allowed solutions.

2.2. Calculate the reaction rate

For given values of $\mathbf{v}_a$ and $\mathbf{v}_b$, the reaction rate per unit volume, time and solid angle is given by

$$r\left(\mathbf{v}_a, \mathbf{v}_b, \mathbf{u}\right) = \frac{n_a n_b}{1 + \delta_{ab}} \left|\mathbf{v}_a - \mathbf{v}_b\right| \frac{{\rm d}\sigma}{{\rm d}\Omega}\left(\mathbf{v}_a, \mathbf{v}_b, \mathbf{u}\right), \tag{5}$$

where $n_{a,b}$ denote the number densities (particles per unit volume) of the respective reactant distributions. The Kronecker delta, δ_{ab}, is included in order to avoid double counting in the case when the reacting particles come from the same distribution. The contribution of each Monte-Carlo event to the reaction rate is therefore given by this expression multiplied by the reactant weights,

$$r_i = w_{a,i} w_{b,i} r\left(\mathbf{v}_{a,i}, \mathbf{v}_{b,i}, \mathbf{u}\right). \tag{6}$$

In order to obtain $\mathrm{d}\sigma/\mathrm{d}\Omega$, the DRESS code uses the parameterizations from [11] for the total cross section and a Legendre polynomial expansion from the ENDF database [12] for the angular dependence. The cross sections are given in the center-of momentum (COM) reference frame, where $\mathbf{p}_a = \mathbf{p}_b$, and are evaluated by Lorentz transforming the relevant four-vectors to the COM frame (the velocity of the COM frame is $\boldsymbol{\beta} = \mathbf{p}_{\mathrm{tot}}/E_{\mathrm{tot}}$). The COM differential cross section is then transformed back into the original reference frame using the Jacobian as given in [13],

$$\frac{\partial\Omega_{\mathrm{CMS}}}{\partial\Omega} = \frac{p_\alpha^2}{\frac{E_{\mathrm{tot}}}{s} p_\alpha^* \left(p_\alpha - E_\alpha \mathbf{u}\cdot\boldsymbol{\beta}\right)}, \tag{7}$$

where the asterisk (*) is used to label COM quantities.

2.3. Generate the spectrum

After N iterations, the result of repeating steps 1, 2 and 3 above is a set of energies $E_{\alpha,i}$ and reaction rates r_i $(i = 1, 2, \ldots N)$. The energy spectrum of particle α is obtained by binning the values according to the energies $E_{\alpha,i}$. The flux of particles with energies between E_j and E_{j+1} is given by the average reaction rate for that bin,

$$R_j = \frac{1}{W} \sum_{i=1}^{N} r_i \theta_{j,i}. \tag{8}$$

In this expression, W denotes the sum of the reactant weights, $\sum_{i=1}^{N} w_{a,i} w_{b,i}$, and $\theta_{j,i}$ is defined to be one if $E_{\alpha,i}$ is in the energy range of interest and zero otherwise. The variance of R_j (σ_R^2) is related to the variance of the terms r_i contributing to the sum (σ_r^2),

$$\sigma_R^2 = \frac{1}{W^2} \sum_{i=1}^{N} \sigma_r^2 = \frac{N}{W^2} \sigma_r^2. \tag{9}$$

Furthermore, σ_r^2 can be estimated from the Monte-Carlo sample as (for large N)

$$\sigma_r^2 = \frac{1}{N}\sum_{i=1}^{N}\left(r_i\theta_{j,i}\right)^2 - \left(\frac{1}{N}\sum_{i=1}^{N} r_i\theta_{j,i}\right)^2 . \tag{10}$$

Hence, the fractional error in each bin is given by

$$e_j = \frac{\sigma_R}{R_j} = \left(\frac{\sum_{i=1}^{N}\left(r_i\theta_{j,i}\right)^2}{\left(\sum_{i=1}^{N} r_i\theta_{j,i}\right)^2} - \frac{1}{N}\right)^{1/2} . \tag{11}$$

This completes the description of the product spectrum calculation.

The DRESS code is written in FORTRAN. Typically, 10^6-10^7 Monte-Carlo particles are required to obtain sub-percent precision. Such a calculation takes about 1-10 seconds on a standard desktop computer. This time could be reduced by parallelizing the code, but this is currently not implemented.

3. Validation

The DRESS code has been tested in several steps. First, the kinematics calculation, equation (4), has been benchmarked against the event generator that is supplied with the ROOT data analysis framework [14, 15]. Given two reactant four-vectors, this module generates two random product four-vectors from the available phase space. As opposed to the DRESS code, it is not possible to select the direction of one of the outgoing particles in ROOT, but it is still possible to compare the results from the two codes by generating events with ROOT and calculate the DRESS result for the corresponding emission direction for one of the products. The results from the two codes are in good agreement; the values obtained for the energy E_α are found to be the same, with an accuracy of about 10 decimal places.

Second, the reaction rate calculation has been compared with the parameterizations of the thermonuclear reactivities for the DT and DD reactions, as given in [11]. The thermonuclear reactivity, commonly denoted by $\langle\sigma v\rangle$, corresponds to the average of the quantity $\sigma\left|\mathbf{v}_a - \mathbf{v}_b\right|$ over reactant distributions in thermal equilibrium, i.e. distributed according to the Maxwellian distribution. Here, σ is the total cross section of the reaction under consideration. The value of $\langle\sigma v\rangle$ is therefore the number of reactions per unit

time and volume divided by the product of the reactant densities and the Kronecker delta term (c.f. equation (5)). The corresponding value is readily obtained from the DRESS code by calculating the energy spectrum of one of the products in the DD and DT reactions, for Maxwellian reactant distributions with $n_a = n_b = 1$, and integrating the result over all energies and emission angles (and taking into account that $\delta_{ab} = 1$ for the DD reaction). A comparison of reactivities obtained from the DRESS code and from the corresponding parameterizations is shown in figure 1, for a range of reactant temperatures. The values obtained from the DRESS code agree well with the parameterized values for all temperatures. The deviation between two values is always smaller than 1 percent, for 10^7 Monte-Carlo particles. However, it can be seen that the deviations between the DRESS results and the parameterized reactivities are significantly larger than the Monte Carlo errors. This is probably due to the fact that the parameterized reactivities are calculated using a detailed R-matrix evaluation of the cross sections, rather than the parameterized cross sections (which are also based on this R-matrix evaluation). This introduces an additional source of discrepancy, apart from the statistical noise.

Third, the calculated spectra can be compared against analytical results. An exact, relativistically correct expression for the DT and DD neutron energy spectra, for Maxwellian reactant distributions, has been derived in [5]. A comparison between DRESS code calculations and the analytical formula is presented in figures 2 and 3, for a selection of temperatures. For each temperature, 100 DRESS simulations were made, with $2 \cdot 10^6$ Monte-Carlo particles for each spectrum. The left column of the figures show a comparison between the average of the DRESS spectra and the analytical result, as well as the difference between the two spectra. The DRESS code results agree well with the analytical expressions. The right column shows a comparison between the average of the Monte-Carlo error (obtained from equation (11)) and the root mean square of the differences between the analytical spectrum and the 100 DRESS spectra. These two estimates of the error are seen to be in good agreement, i.e. in this case the differences between the DRESS calculations and the analytical result is consistent with what is expected from Monte-Carlo statistics.

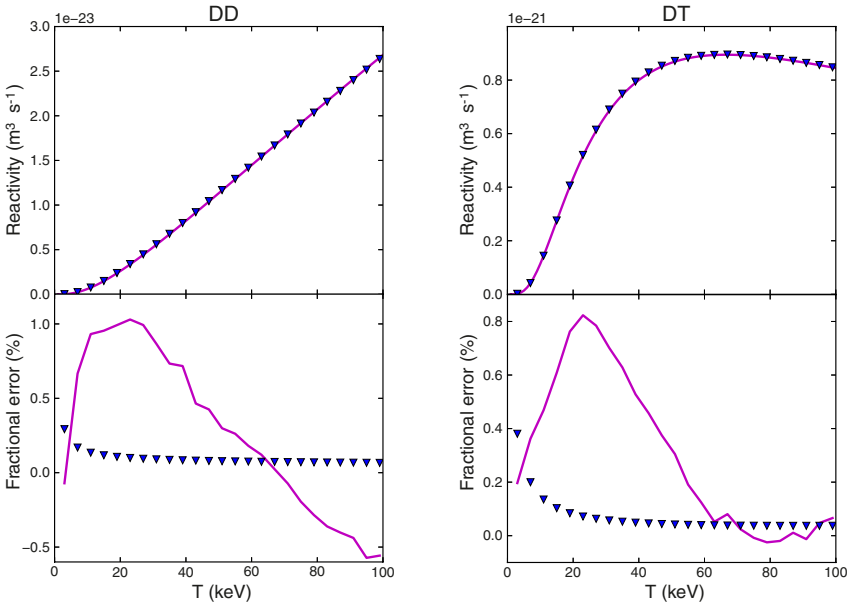

Figure 1: Comparison of parameterized thermonuclear reactivities (magenta line) for the DD (left) and DT (right) fusion reactions with the corresponding values obtained from DRESS code calculations (blue triangles). The top panel shows the calculated reactivities and the bottom panel shows the fractional difference between the parameterizations and the DRESS code results (magenta line) as well as the statistical uncertainty estimated from the Monte-Carlo statistics (blue triangles).

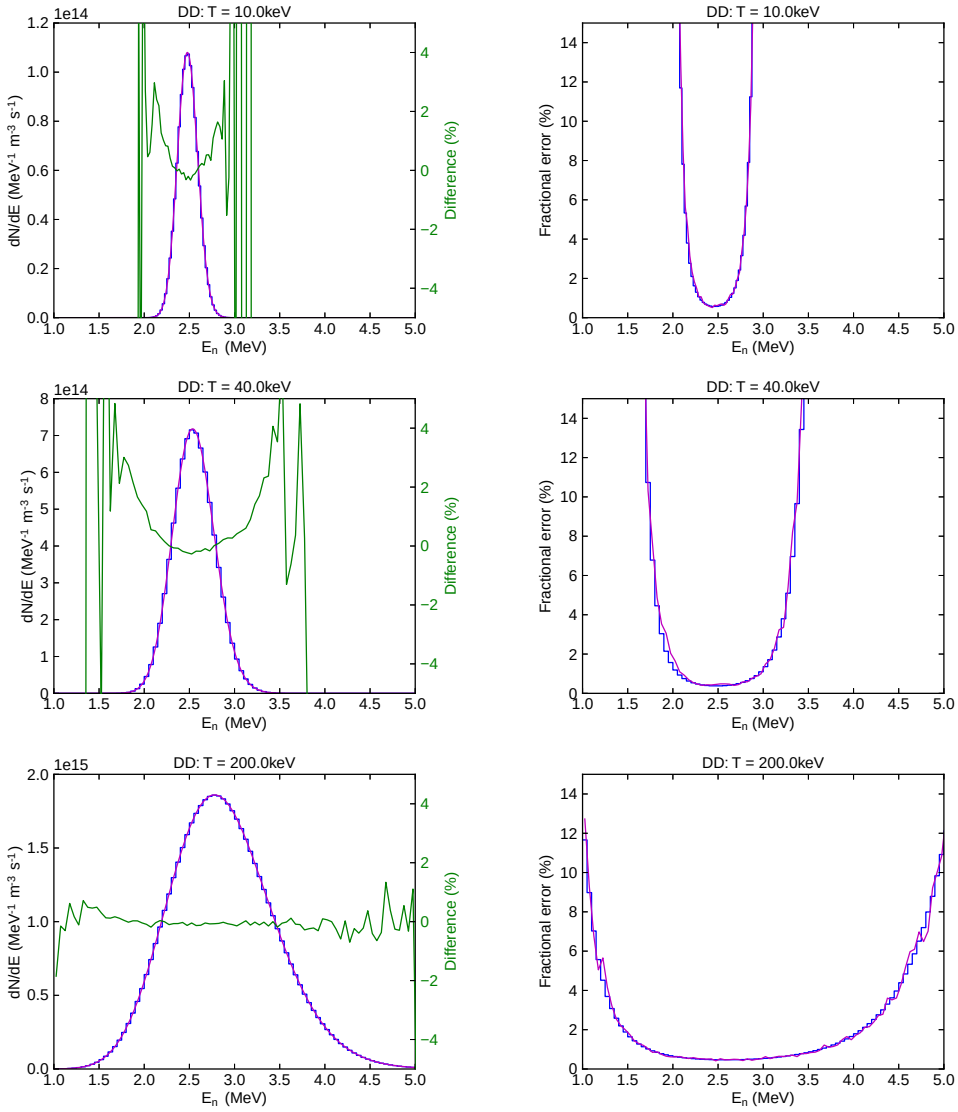

Figure 2: Neutron energy spectra from Maxwellian reactant distributions of different temperatures, for the DD fusion reaction. The step plots are DRESS calculations and the magenta lines are analytical results from [5]. The left panel shows the spectra and the difference between them (green line). The right panel shows the average fractional difference between the analytical spectrum and the DRESS code result (magenta line) as well as the statistical uncertainty in the DRESS code result estimated from the Monte-Carlo statistics (blue steps). More details about the plots are given in the main text.

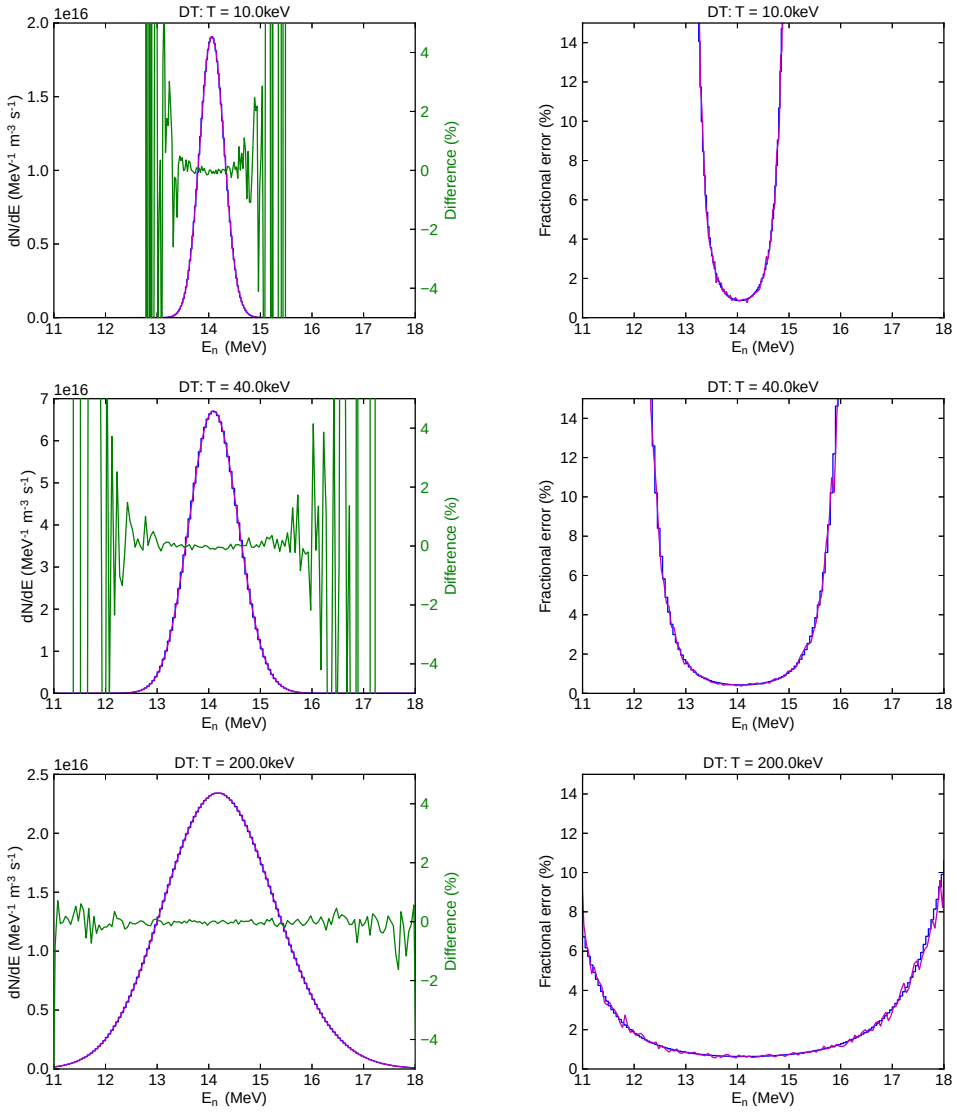

Figure 3: Neutron energy spectra from Maxwellian reactant distributions of different temperatures, for the DT fusion reaction. The step plots are DRESS calculations and the magenta lines are analytical results from [5]. The left panel shows the spectra and the difference between them (green line). The right panel shows the average fractional difference between the analytical spectrum and the DRESS code result (magenta line) as well as the statistical uncertainty in the DRESS code result estimated from the Monte-Carlo statistics (blue steps). More details about the plots are given in the main text.

4. Example results

Several DRESS code calculations that illustrate various properties of DD and DT neutron spectra are presented in this section. The purpose is to demonstrate the various capabilities of the DRESS code; all the properties of the DD and DT reactions discussed here are well known from previous work.

Consider first two mono-energetic beams, both with a particle density of $1 \cdot 10^{19}$ m^{-3}, organized in such a way that the reference frame of observation coincides with the COM frame. The total energy E_{tot} is put to 250 keV. In the COM frame the product energies are determined solely by E_{tot} and the particle masses, i.e. independent of the emission direction (c.f. equation (3), with $\mathbf{p}_{\text{tot}} = \mathbf{0}$). The calculated neutron rate and neutron energy as a function of emission angle is shown in figure 4, for both the DD and DT reactions. The emission angle is defined as the angle between the incoming deuteron and the outgoing neutron. It is seen that the DD neutron emission is anisotropic in the COM frame, which reflects the DD differential cross section in this reference frame. In contrast, the DT cross section is almost completely isotropic at this energy. Figure 4 also shows the corresponding plots in the reference frame where one of the particles (the triton for the DT case) is at rest, commonly referred to as the LAB frame. In this case the angular distribution of the neutron emission has changed, since the COM cross sections are modified by the Jacobian given in equation (7). Furthermore, the neutron energy now depends on the emission angle, through the term $\mathbf{p}_{\text{tot}} \cdot \mathbf{u}$ in equation (4), which is also illustrated in figure 4.

Next, consider a mono-energetic beam of 500 keV deuterons in a uniform, cold magnetized D plasma. The pitch angles of the beam ions are taken to be 90 degrees. The density of both the beam and background distributions are $1 \cdot 10^{19}$ m^{-3}. The neutron spectrum is calculated for emission directions perpendicular and parallel to the magnetic field, respectively. Due to the Larmor gyration of the beam ions, the neutron spectrum for the perpendicular emission will get contributions from reactions involving beam ions traveling in all different directions compared to the emission direction, ranging from completely parallel ($\mathbf{p}_{\text{tot}} \cdot \mathbf{u} = p_{\text{tot}}$) to completely anti-parallel ($\mathbf{p}_{\text{tot}} \cdot \mathbf{u} = -p_{\text{tot}}$) . Since a 500 keV beam of deuterons reacting with a stationary D target corresponds to a COM energy of 250 keV, the neutron spectrum for this case will essentially be the sum of the LAB neutron energies for different emission angles shown in figure 4. The result is shown in the left panel of figure 5. The situation is different if the emission direction is parallel to the magnetic

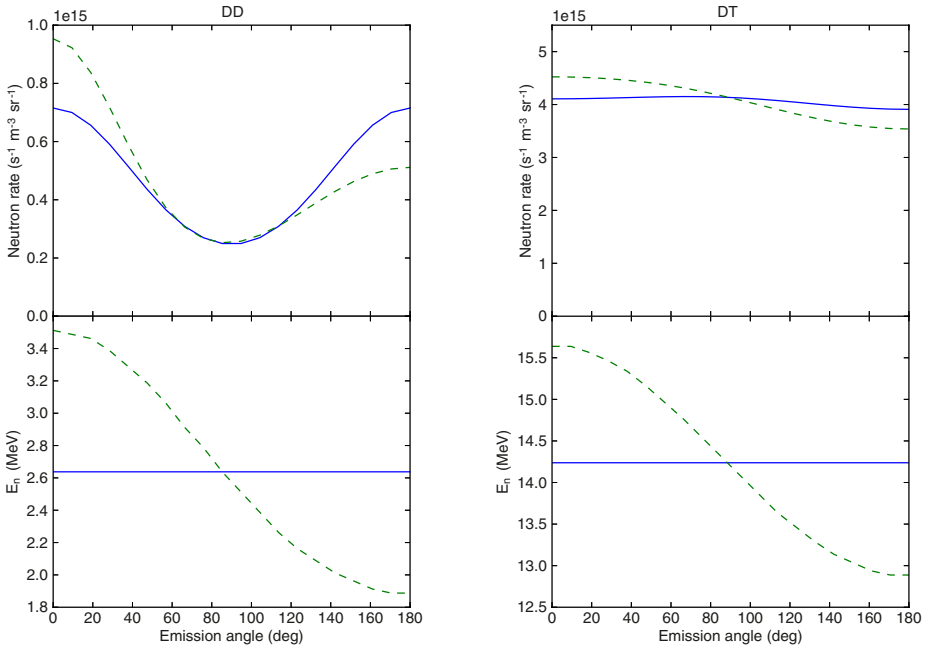

Figure 4: The top panel shows the calculated neutron rate from two colliding mono-energetic beams as a function of emission angle in the COM frame (blue, solid line) and in the LAB frame (green dashed line), for DD (left) and DT (right) fusion reactions with a COM energy of 250 keV. The emission angle is defined as the angle between the incoming deuteron and the outgoing neutron. The bottom panel shows the neutron energy at the corresponding emission angle.

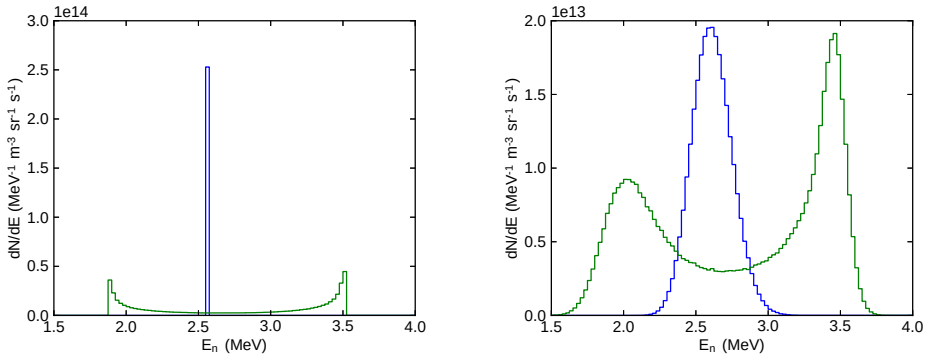

Figure 5: DD neutron spectra for a 500 keV mono-energetic D population in a magnetized D plasma, for an emission angle perpendicular (green) and parallel (blue) to the magnetic field. The pitch angles of the beam ions are 90 degrees. In the left panel the background plasma has zero temperature and in the right panel the temperature is 20 keV.

field. In this case only reactions with $\mathbf{p}_{\mathrm{tot}} \cdot \mathbf{u} = 0$ contribute to the neutron spectrum, which is therefore mono-energetic, as shown in the same figure.

Next, the effect of a finite temperature of the background plasma in the previous example is considered. The resulting spectra are shown in the right panel of figure 5, for a plasma temperature of 20 keV. The qualitative picture is the same as in the cold plasma case, but the spectral features are broadened due to the thermal motion of the ions.

Finally, a spectrum from a more realistic fuel ion distribution is shown in figure 6. An NBI slowing down distribution obtained from a simulation of a JET-like plasma, using the plasma transport code TRANSP [16], is considered. The injection energy is about 100 keV and due to the directionality of the beams the resulting slowing down distribution is highly anisotropic in the pitch angle coordinate, as seen from the left panel of figure 6. This distribution can be used by the DRESS code (together with a Maxwellian background distribution) in order to calculate the beam-thermal and beam-beam neutron spectra. The result is shown in the right panel of figure 6. The beam-thermal spectrum has similar features as the more idealized beam-target spectra already studied (c.f. figure 5) and the beam-beam spectrum is Gaussian-like, with a broadening related to the spread in the energy of the slowing down distribution.

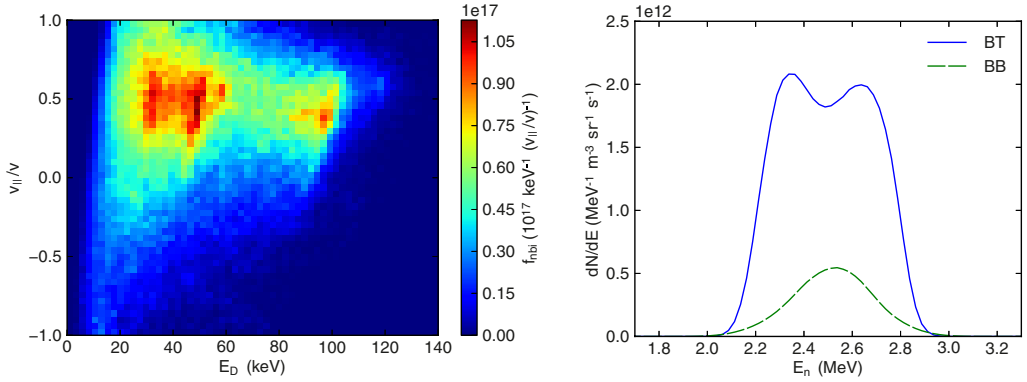

Figure 6: The left panel shows an example of a D distribution of the type commonly found in NBI heated tokamak plasmas. In the right panel the calculated beam-thermal (BT) and beam-beam (BB) neutron spectra are shown, for an emission direction perpendicular to the plasma magnetic field. The temperature and density of the background plasma is 4.9 keV and $3.4{\cdot}10^{19}$ m^{-1}, respectively.

5. Summary and outlook

The Directional Relativistic Spectrum Simulator (DRESS) code allows for the calculation of reaction product spectra from arbitrary reactant distributions. The code is currently setup to calculate spectra from the DD and DT fusion reactions, but any other reaction can be simulated as well, by changing the cross section and the relevant particle masses. The code has been benchmarked against the kinematics module of the ROOT data analysis framework [14, 15]. It has been validated against an analytical expression for the DD and DT neutron spectra from Maxwellian reactant distributions [5] and against parameterized values of thermonuclear fusion reactivities [11].

The DRESS code is currently used for the analysis and interpretation of neutron spectrometry and neutron profile measurements at the JET and MAST tokamaks. The code can be coupled to a detailed 3-dimensional model of the viewing cone of a given measuring instrument. This allows for the calculation of the energy spectra expected to be seen by a given instrument, using spatially resolved reactant distributions given e.g. by the plasma transport code TRANSP [16]. This synthetic diagnostic framework will be described in a future paper.

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