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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.

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 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 [1–3]. 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 [7–9]. 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

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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 2–4 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

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

Rearranging and squaring this equation gives

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

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

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

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

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

where

$$A = \frac{s + m_\alpha^2 - m_\beta^2}{2E_{\mathrm{tot}}},$$

$$B = \frac{\mathbf{p}_{\mathrm{tot}}}{E_{\mathrm{tot}}} \cdot \mathbf{u}.$$

Eq. (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_{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

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

where $n_{a,b}$ denotes 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 1–3 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),

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