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Note

A New Expansion Method for Computing $\overline{\sigma v}$ for Reactant Distribution Functions*

1. Introduction

Fusion reactor studies [1, 2] involve computation of the reaction rate for two reacting species a and b:

$$R = \int d\mathbf{v} \int d\mathbf{v}' \, f_a(\mathbf{v}) \, f_b(\mathbf{v}') \, \sigma(u) \, u,$$

where R is the number of reactions per unit volume per unit time, f_a and f_b are the distribution functions, σ is the reaction cross section, and u is the relative velocity

$$u = | \mathbf{v} - \mathbf{v}' |.$$

It is often convenient to write

$$R = n_a n_b \overline{\sigma v},$$

where n_a and n_b are the densities given by

$$n_i = \int f_i(\mathbf{v}) \, d\mathbf{v} \qquad (i = a, b)$$

and $\overline{\sigma v}$ is the reaction rate parameter, a quantity which depends on the form of the normalized distribution functions:

$$\overline{\sigma v} = \frac{1}{n_a n_b} \int d\mathbf{v} \int d\mathbf{v}' \, f_a(\mathbf{v}) \, f_b(\mathbf{v}') \, \sigma(u) \, u. \tag{1}$$

In this note we present a very fast method [Eq. (8)] for computing $\overline{\sigma v}$ for distributions which are independent of the azimuthal angle ϕ in spherical coordinates. The method is based on an expansion in Legendre polynomials. Hence, it can be very conveniently adapted to existing Fokker–Planck codes in which Legendre expansions of the distribution functions are already computed to facilitate evaluation of the collision operator [2]. This method is compared with two others, and found to be the most economical for given accuracy.

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2. Derivation of the Method

Assume distribution functions $f_a(v, \theta)$ and $f_b(v, \theta)$, where v and θ are the usual radial and polar angle variables in spherical coordinates in velocity space. To derive the formula for $\overline{\sigma v}$ which is most convenient for computation, it is necessary to make a change of variables in performing the integration over $\mathbf{v}'$ in Eq. (1). The new variables are the coordinates v', θ_{12}, and ϕ_{12} in a spherical coordinate system in which the polar axis is along the vector $\mathbf{v}$. (See Fig. 1) The azimuthal angle ϕ_{12} is

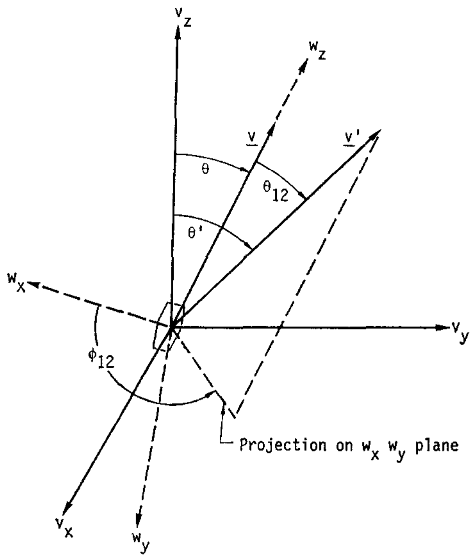

FIG. 1. Coordinate system. The axes labeled w_x, w_y, and w_z are the Cartesian axes in the new coordinate system used to represent $\mathbf{v}'$. The w_x-axis lies in the w_z-v_z plane.

measured from the plane which includes $\mathbf{v}$ and the polar axis in the original (v, θ, ϕ) coordinate system, and θ_{12} is simply the angle between $\mathbf{v}$ and $\mathbf{v}'$.

In terms of these coordinates, (1) becomes

$$\overline{\sigma v} = \frac{1}{n_a n_b} \int_0^\infty v^2\, dv \int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi\, f_a(v, \theta)$$
$$\times \int_0^\infty v'^2\, dv' \int_0^\pi \sin\theta_{12}\, d\theta_{12} \int_0^{2\pi} d\phi_{12}\, f_b(v', \theta')\, \sigma(u)\, u. \tag{2}$$

Note that the angle θ' between $\mathbf{v}'$ and the original polar axis is a function of θ, θ_{12}, and ϕ_{12}. It can be shown that

$$\cos\theta' = \cos\theta\cos\theta_{12} + \sin\theta\sin\theta_{12}\cos\phi_{12}. \tag{3}$$

Note also that the relative velocity is a function only of v, v', and θ_{12}:

$$u = (v^2 + v'^2 - 2vv' \cos \theta_{12})^{1/2}, \tag{4}$$

and that the integration over ϕ is trivial.

The distribution functions are expressed as a Legendre series:

$$f_i(v, \theta) = \sum_{l=0}^{\infty} F_{il}(v)\, P_l(\cos \theta) \qquad (i = a, b), \tag{5}$$

where

$$F_{il}(v) = \frac{2l+1}{2} \int_0^{\pi} \sin \theta \, d\theta \, P_l(\cos \theta)\, f_i(v, \theta).$$

This expansion is now inserted in Eq. (2) for f_a and f_b, and the addition theorem for spherical harmonics [3]

$$P_n(\cos \theta') = \sum_{m=-n}^{n} \frac{(n-m)!}{(n+m)!} P_n{}^m(\cos \theta)\, P_n{}^m(\cos \theta_{12}) \cos m\phi_{12}$$

is used to evaluate the Legendre functions in the expansion of f_b. The result is

$$\begin{aligned} \overline{\sigma v} = {} & \frac{2\pi}{n_a n_b} \int_0^{\infty} v^2\, dv \int_0^{\pi} \sin \theta \, d\theta \sum_{l=0}^{\infty} F_{al}(v)\, P_l(\cos \theta) \\ & \times \int_0^{\infty} v'^2\, dv' \int_0^{\pi} \sin \theta_{12}\, d\theta_{12}\, \sigma(u)\, u \sum_{n=0}^{\infty} F_{bn}(v') \\ & \times \sum_{m=-n}^{n} \frac{(n-m)!}{(n+m)!} P_n{}^m(\cos \theta)\, P_n{}^m(\cos \theta_{12}) \int_0^{2\pi} d\phi_{12} \cos m\phi_{12} . \end{aligned}$$

Noting that the ϕ_{12} integration is nonzero only if $m = 0$, so that only $P_n{}^0 = P_n$ appears, and using the orthogonality of the Legendre polynomials on the θ domain, we have

$$\begin{aligned} \overline{\sigma v} = {} & \frac{8\pi^2}{n_a n_b} \sum_{l=0}^{\infty} \frac{1}{2l+1} \int_0^{\infty} v^2\, dv\, F_{al}(v) \int_0^{\infty} v'^2\, dv'\, F_{bl}(v') \\ & \times \int_0^{\pi} \sin \theta_{12} P_l(\cos \theta_{12})\, \sigma(u)\, u\, d\theta_{12} , \end{aligned} \tag{6}$$

where u is obtained from Eq. (4).

This formula for $\overline{\sigma v}$ is evaluated by truncating the series at $l = L$, and performing the three integrations numerically. The Legendre coefficients F_{al} and F_{bl} are given on a common velocity mesh v_j ($j = 1, 2, \ldots, J$), and a quadrature formula

$$\int_0^{\infty} f(v)\, dv \cong \sum_{j=1}^{J} c_j f(v_j)$$

is assumed. Similarly, we use a K-point quadrature formula for integration over θ:

$$\int_0^{\pi} \sin\theta\, f(\theta)\, d\theta \cong \sum_{k=1}^{K} \hat{c}_k f(\theta_k).$$

(The trapezoidal rule has been used throughout this work for purposes of compatibility with existing codes [2]. The conservative difference scheme used in these codes requires trapezoidal integration for particle conservation. Better accuracy in the $\overline{\sigma v}$ calculation could no doubt be achieved with higher-order integration formulas.) The numerical formula for the θ_{12} integral in Eq. (6) at v_j and $v_{j'}$ is then

$$A_{jj'l} = \sum_{k=1}^{K} P_l(\cos\theta_{12k})\, \sigma(u)\, u\hat{c}_k\,, \tag{7}$$

with u a function of v_j, $v_{j'}$, and θ_{12k}.

We then write

$$\overline{\sigma v} \cong \frac{1}{n_a n_b} \sum_{j=1}^{J} \sum_{j'=1}^{J} \sum_{l=0}^{L} F_{ajl} F_{bj'l} I_{jj'l}\,, \tag{8}$$

where

$$F_{ijl} = F_{il}(v_j) \qquad (i = a, b)$$

and

$$I_{jj'l} = \frac{8\pi^2}{2l+1} v_j^2 v_{j'}^2 c_j c_{j'} A_{jj'l}\,. \tag{9}$$

Hence, the five-dimensional integral which appears after performing the trivial ϕ integration in Eq. (2) actually reduces to a triple sum, which can be performed very rapidly.

It is important to note that the coefficients $I_{jj'l}$ do not involve the distribution functions. Hence, they need be evaluated only once for any velocity mesh. In other words, they are evaluated only at the beginning of a calculation in which distribution functions and reaction rates are followed in time. Making use of the symmetry

$$I_{jj'l} = I_{j'jl}$$

also saves both computer time and storage. The amount of storage required for these coefficients is

$$\frac{J(J+1)(L+1)}{2}$$

locations. The computer time required for the initial calculation of the $I_{jj'l}$ is approximately

$$(4.5 \times 10^{-6})(J)(J+1)(K)(L+1) \text{ seconds}$$

on a CDC 7600 computer. Each time that Eq. (8) is computed requires approximately

$$2.5 \times 10^{-6}(K + \tfrac{2}{3}J)(L + 1)(J) \text{ seconds}.$$

Note that this expression also includes the time required to compute the coefficients F_{ijl}. The setup time, computation time, and storage requirement are given in Table I for a typical run with $J = 61$, $K = 21$, and $L = 4$.

TABLE I

Setup Times, Computation Times, and Storage Requirements for the Three Methods when Applied to Distribution Function Arrays Dimensioned 61 × 21[a]

Method	Time to precompute coefficients (sec)	Time to compute $\overline{\sigma v}$(sec)	Storage required
Fast (3-D) Legendre	1.8	0.05	9455
Slower (4-D) Legendre	162	0.09	17019
Trapezoidal rule (5-D)	Insignificant	85	Insignificant

[a] The Legendre expansions were truncated at $L = 4$. Setup time and storage requirements for the trapezoidal rule are only those required to define the coefficients for one-dimensional integration over v, θ and ϕ.

3. Other Schemes

A second method [4] also involves the expansion of the reacting distribution functions in Legendre polynomials; however, in this case the vector $\mathbf{v}'$ receives no special treatment and is represented as (v', θ', ϕ') relative to the same (x, y, z) axis as the vector $\mathbf{v}$. We obtain a relation

$$\overline{\sigma v} = \frac{2\pi}{n_a n_b} \int_0^\infty v^2\, dv \int_0^\infty v'^2\, dv' \int_0^\pi \sin\theta\, d\theta \times \int_0^\pi \sin\theta'\, d\theta'\, f_a(v, \theta)\, f_b(v', \theta') \int_0^{2\pi} d\phi\, \sigma(u)\, u,$$

where

$$u = [v^2 + v'^2 - 2vv'(\cos\theta \cos\theta' + \sin\theta \sin\theta' \cos\phi)]^{1/2}.$$

Aside from expanding the distribution functions in a Legendre series, we must also expand the integral over ϕ in a double Legendre series. One obtains an expression of the form

$$\overline{\sigma v} = \frac{1}{n_a n_b} \sum_{j=1}^{J} \sum_{j'=1}^{J} \sum_{l=0}^{L} \sum_{\substack{l'=0 \\ l+l'\,\text{even}}}^{L} F_{ajl} F_{bj'l'} I_{jj'll'}\,.$$

The computation is then streamlined by making use of the symmetries

$$I_{jj'll'} = I_{j'jll'} ,$$
$$I_{jj'll'} = I_{jj'l'l} ,$$

and the odd-even parity of the Legendre functions. The resulting array of coefficients requires

$$J(J + 1)(L/2 + 1)^2/2$$

storage locations when L is even. For the case $L = 4$, storage requirements are 80 % greater than for the preceding method. Furthermore, these coefficients are more expensive to compute, involving on the order of 90 times the computer time for a θ mesh of 21 points. Referring to Table I, we note that each computation of $\overline{\sigma v}$ requires about 0.09 seconds for the mesh described above as opposed to 0.05 seconds for the more efficient method (since there are 80 % more coefficients and resulting operations.)

Using the fusion reaction cross section of Kuo–Petravic *et al.* [5], these two methods and a straightforward five-dimensional trapezoidal integration procedure were compared for a variety of distribution functions, including highly anisotropic (θ-dependent) cases. The answers differed by less than 1 % for the values of J, K, and L mentioned previously. To emphasize the savings resulting from use of Legendre expansions for this type of calculation, we note that about 85 seconds were required for each computation of $\overline{\sigma v}$ employing the trapezoidal integration with the above mesh. (See Table I.) Hence, the computation times for the two Legendre methods are insignificant. Even the setup time for the fast method is much shorter. An interesting but moot point is that it takes longer to perform *one* $\overline{\sigma v}$ computation via the longer four-dimensional Legendre method than via the trapezoidal rule, because of the setup time.

4. Concluding Remarks

The fast Legendre expansion method has been applied successfully to counter-streaming (hence anisotropic) deuterium-tritium distributions (see Ref. 6.) It has been incorporated in Fokker–Planck codes in which the fusion reaction rate is followed in order to provide source terms for reaction products (e.g., alpha-particles.)

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