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An efficient nonclassical quadrature for the calculation of nonresonant nuclear fusion reaction rate coefficients from cross section data

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ABSTRACT

Nonclassical quadratures based on a new set of half-range polynomials, $T_n(x)$, orthogonal with respect to $w(x) = e^{-x-b/\sqrt{x}}$ for $x \in [0, \infty)$ are employed in the efficient calculation of the nuclear fusion reaction rate coefficients from cross section data. The parameter $b = B/\sqrt{k_BT}$ in the weight function is temperature dependent and B is the Gamow factor. The polynomials $T_n(x)$ satisfy a three term recurrence relation defined by two sets of recurrence coefficients, α_n and β_n. These recurrence coefficients define in turn the tridiagonal Jacobi matrix whose eigenvalues are the quadrature points and the weights are calculated from the first components of the eigenfunctions. For nonresonant nuclear reactions for which the astrophysical function can be expressed as a lower order polynomial in the relative energy, the convergence of the thermal average of the reactive cross section with this nonclassical quadrature is extremely rapid requiring in many cases 2–4 quadrature points. The results are compared with other libraries of nuclear reaction rate coefficient data reported in the literature.

1. Introduction

The thermal reaction rate coefficients for nuclear reactions are calculated from the appropriate collision cross sections averaged over a Maxwellian relative energy distribution. The development of nuclear fusion reactors requires the temperature dependence of nuclear reaction rate coefficients [1,2] for the isotopes of hydrogen and helium, namely D(d, p)T, D(d, n)^{3}He, T(d, n)^{4}He, ^{3}He(d, p)^{4}He and other reactions [3]. These reactions are also the basis for models of primordial or big bang nucleosynthesis [4–6] in conjunction with constraints imposed by observations of the cosmic microwave background [7]. These kinetic data are also required to model stellar astrophysics such as the Sun and other stars including supernovae [8,9]. There exist several different libraries of reaction rate coefficient data that include empirical fits of rate coefficients versus temperature [4,10,11] as well as tables that require interpolations [12,13] and other databases [14]. An efficient and accurate representation of the temperature dependence of the nuclear reaction rate coefficients from cross section data is an important endeavor.

The objective of this paper is to report on a novel efficient numerical quadrature to calculate exactly the temperature dependence of the nuclear rate coefficients from given nonresonant cross section data. Specific nonclassical quadratures have been used in numerous pseudospectral solutions of integral and differential equations in numerous fields and in particular in kinetic theory [15,16] and quantum mechanics [15,17–23]. There have also been many discussions of quadrature rules [24,25] and several methods specifically designed for applied problems [26].

The nuclear reactive cross sections are generally expressed in terms of the astrophysical factor, $S(E)$, which is most often written as a low order power series in the relative energy, E. The method proposed in this paper is based on the exact evaluation of the rate coefficient, $k(T)$, defined by Eq. (2), with a quadrature defined by a set of nonclassical polynomials orthogonal with respect to the weight function, $w_1(x) = \exp(-x - b/\sqrt{x})$, where $b = B/\sqrt{k_BT}$, B is the Gamow factor and k_B is the Boltzmann constant [2]. This quadrature provides an exact result for nonresonant nuclear reactions with $S(E)$ expressed as a lower order polynomial in the relative energy E. The weight function $w_1(x)$ can be recognized as the integrand in the Maxwellian average of the cross section for which $S(E) = s_0$ is independent of E. An often used approximation in this simplest case is to expand the argument of the exponential in $w_1(x)$ up to quadratic terms which gives a Gaussian approximation to the integrand which can be integrated analytically. This provides a first order estimate for the reactive rate coefficient [2,22].

For $S(E) = \sum_{n=0}^{N} s_nE^n$, the rate coefficient, $k(T)$, can be expressed in terms of the moments of $w_1(x)$. With the asymptotic

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expansion of these moments in terms of $T^{\frac{1}{3}}$ [27], the rate coefficient can be expressed as

$$k_{(asymp)}(T) \approx A_1 e^{-A_2/T^{\frac{1}{3}}}\left[1+\sum_{m=1}^{M} C_m T^{\frac{m}{3}}\right]\Big/ T^{\frac{2}{3}} \quad (1)$$

where the coefficients A_1, A_2 and C_m are calculated from the s_n coefficients. This analytic expression for $k_{asmyp}(T)$ is often used but with the coefficients determined with a least squares fitting procedure so that the final results are not exact [4,6,28]. An alternate approach is based on the asymptotic expansion of the moments of the weight function, Eq. (6), in powers of $1/\tau$ where $\tau = 3(\frac{b}{2})^{\frac{2}{3}}$ as defined in Section 2. The coefficients in Eq. (1) are then evaluated in a theoretical manner [27,29]. Any round-off errors that may occur in the use of Eq. (1) can be significantly reduced if $k_{asymp}(T)$ is evaluated as a nested sum.

The new nonclassical quadrature based on the weight function $w_1(x), x \in [0,\infty)$ is presented in Section 2. Section 3 provides a comparison of the quadrature evaluated rate coefficients with analytic fits reported in the literature, such as Eq. (1), as well as with other libraries of reaction rate data. Section 4 provides a summary of the results.

2. A quadrature based on nonclassical polynomials

The reaction rate coefficient, $k(T)$, versus temperature, T, is given by the average of the reactive cross section, $\sigma(E)$, with the Maxwellian distribution of relative energies, that is,

$$k(T) = \sqrt{\frac{8}{\pi\mu}}\frac{1}{(k_BT)^{3/2}}\int_0^\infty E e^{-E/k_BT}\sigma(E)dE. \quad (2)$$

The reactive cross sections are often written in terms of the astrophysical factor [2], $S(E)$, and the cross section is given by

$$\sigma(E) = \frac{S(E)}{E}e^{-B/\sqrt{E}}, \quad (3)$$

where $B = 31.29106 Z_1 Z_2\sqrt{\mu}$ in $\sqrt{\text{keV}}$ is the Gamow factor [2], Z_1 and Z_2 denote the nuclear charges of the two nuclei and $\mu = m_1m_2/(m_1+m_2)$ is the reduced mass in atomic mass units (amu) of the reacting nuclei [1,2]. There are numerous analytical representations of the energy dependence of $S(E)$ for different nuclear reactions [3,4,10]. For nonresonant reactions, the astrophysical factor can be represented as a power series in the relative energy E, that is,

$$S(E) = \sum_{n=0}^{N} s_n E^n. \quad (4)$$

With the substitution of Eq. (4) into Eq. (2), the rate coefficient can be written as

$$k(T) = \sqrt{\left(\frac{8}{\pi\mu k_BT}\right)}\sum_{n=0}^{N} s_n (k_BT)^n I_n(b). \quad (5)$$

With the transformation to reduced energy, $x = E/k_BT$, the dimensionless integrals in Eq. (5) are given by

$$I_n(b) = \int_0^\infty x^n e^{-x-b/\sqrt{x}}dx, \quad (6)$$

where $b = B/\sqrt{k_BT}$ is temperature dependent.

A low order estimate of the rate coefficient is obtained for constant $S(E) = s_0$, for which the integrand in Eq. (6) with $n = 0$ exhibits an extremum. The standard first order approximation for $I_0(b)$ [2,22,30] involves the expansion of the argument of the exponential, $f(x) = x + b/\sqrt{x}$, up to quadratic terms about the position of the maximum evaluated as $x_m = (b^2/4)^{\frac{1}{3}}$. In terms of $\tau = 3(\frac{b}{2})^{\frac{2}{3}} = 3(\frac{B}{2\sqrt{k_B}})^{\frac{2}{3}}T^{-\frac{1}{3}}$, this first order approximation yields a Gaussian integrand and $I_0(b) \approx 2\sqrt{\pi\tau}e^{-\tau}/3$. The rate coefficient with this approximation is

$$k(T) \approx A_1 e^{-A_2/T^{\frac{1}{3}}}/T^{\frac{2}{3}}, \quad (7)$$

where

$$A_1 = \frac{2s_0}{3}\sqrt{\frac{8A_2}{\mu k_BT}}, \quad (8)$$

$$A_2 = 3\left(\frac{B}{\sqrt{k_B}}\right)^{\frac{2}{3}}.$$

The peak of the Gaussian approximation to $f(x)$ occurs at the dimensional energy referred to as the Gamow energy or the Gamow peak given by $E_G = (Bk_BT/2)^{\frac{2}{3}}$.

The principal objective of this paper is to introduce a numerical evaluation of integrals of the form in Eq. (2) based on a quadrature defined in terms of nonclassical polynomials, $T_n(x)$, orthogonal according to

$$\int_0^\infty e^{-x-b/\sqrt{x}}T_n(x)T_m(x)dx = \delta_{nm}. \quad (9)$$

The weight function $w_1(x) = e^{-x-b/\sqrt{x}}$ is precisely the integrand for $I_0(b)$ in Eq. (6). With the quadrature to be defined, we will show that the integrals $I_n(b)$ can be computed exactly with $(N+1)/2$ quadrature points and weights. Since $S(E)$ for many nuclear reactions is a low order polynomial, a very small number of quadrature points and weights will be required.

The nonclassical $T_n(x)$ polynomials satisfy a general three term recurrence relation

$$xT_n(x) = \sqrt{\beta_{n+1}}T_{n+1}(x) + \alpha_nT_n(x) + \sqrt{\beta_n}T_{n-1}(x) \quad (10)$$

where α_n and β_n are the recurrence coefficients [22,31]. The quadrature points and weights in the quadrature algorithm

$$\int_0^\infty e^{-x-b/\sqrt{x}}F(x)dx \approx \sum_{i=1}^{N} w_iF(x_i) \quad (11)$$

are computed from the diagonalization of the $N \times N$ Jacobi matrix [22], given by

$$\mathbf{J} = \begin{pmatrix} \alpha_0 & \sqrt{\beta_1} & 0 & 0 & \dots & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & 0 & \dots & 0 \\ 0 & \sqrt{\beta_2} & \alpha_2 & \sqrt{\beta_3} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & 0 & 0 & \sqrt{\beta_N} & \alpha_N \end{pmatrix}. \quad (12)$$

The Jacobi matrix can be recognized as the matrix representation of the coordinate operator. The quadrature points are the eigenvalues of $\mathbf{J}$ and the weights are obtained from the first component of the ith eigenvector [22,32,33]. The quadrature algorithm, Eq. (11), is exact with N quadrature points for $F(x)$ a polynomial of degree 2N − 1 [22,32,33].

If the three term recurrence relation, Eq. (10), is multiplied by $T_n(x)$ and integrated, the orthogonality condition, Eq. (9), gives

$$\alpha_n = \int_0^\infty e^{-x-b/\sqrt{x}}xT_n^2(x)dx. \quad (13)$$

The recurrence relation for the monic polynomials, with the coefficient of x^N set to unity is

$$q_{n+1}(x) = (x-\alpha_n)q_n(x) - \beta_nq_{n-1}(x), \quad (14)$$