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An accurate analytic representation of the temperature dependence of nonresonant nuclear reaction rate coefficients

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HIGHLIGHTS

- The development of an asymptotic representation for the temperature dependence of the reactive rate coefficient for nonresonant reactions.
- Comparison of the results with other fitting procedures by several authors.
- The potential application to many other nuclear reactions not considered in the present manuscript.

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ABSTRACT

There has been intense interest for several decades by different research groups to accurately model the temperature dependence of a large number of nuclear reaction rate coefficients for both light and heavy nuclides. The rate coefficient, $k(T)$, is given by the Maxwellian average of the reactive cross section expressed in terms of the astrophysical factor, $S(E)$, which for nonresonant reactions is generally written as a power series in the relative energy E. A computationally efficient algorithm for the temperature dependence of nuclear reaction rate coefficients is required for fusion reactor research and for models of nucleosynthesis and stellar evolution. In this paper, an accurate analytical expression for the temperature dependence of nuclear reaction rate coefficients is provided in terms of $\tau = 3(b/2)^{\frac{2}{3}}$ or equivalently, $T^{-\frac{1}{3}}$, where $b = B/\sqrt{k_B T}$, B is the Gamow factor and k_B is the Boltzmann constant. The methodology is appropriate for all nonresonant nuclear reactions for which $S(E)$ can be represented as a power series in E. The explicit expression for the rate coefficient versus temperature is derived with the asymptotic expansions of the moments of $w(E) = \exp(-E/k_B T - B/\sqrt{E})$ in terms of τ. The zeroth order moment is the familiar Gaussian approximation to the rate coefficient. Results are reported for the representative reactions D(d, p)T, D(d, n)^{3}He and ^{7}Li(p, α)α and compared with several different fitting procedures reported in the literature.

1. Introduction

There has been an ongoing interest for decades in the efficient and accurate representation of the temperature dependence of a large number of nuclear reactions for both light and heavy nuclides [1–4]. The reaction rate coefficient, $k(T)$, can be calculated from the appropriate collision cross section averaged over a Maxwellian relative energy distribution at temperature T. The development of nuclear fusion reactors requires the temperature dependence of nuclear reaction rate coefficients [5,6] for reactions that involve the isotopes of hydrogen and helium, namely D(d,p)T, D(d, n)^{3}He, T(d, n)^{4}He,

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^{3}He(d, p)^{4}He and others [7]. These reactions are also the basis for models of primordial or big bang nucleosynthesis [3,8–11], constrained by observations of the cosmic microwave background [12]. Kinetic data are also required to model stellar astrophysics [13–16] including supernovae [17,18]. In many applications, a large complex reaction network [19,20] is required and coupled to the hydrodynamics and radiative properties of the stellar models. An accurate and efficient representation of $k(T)$ versus T is important. There exist several different libraries of reaction rate data that include empirical fits of rate coefficients versus temperature [2,3,21,22] as well as tables that require interpolations [19,23] and other databases [24]. An efficient and accurate representation of the temperature dependence of the nuclear reaction rate coefficients from cross section data is an important endeavor. Coc et al. [8] point to the need of accurate representations of nuclear reaction rate coefficients for simulations of big bang nucleosynthesis and estimations of the deuterium abundance [25] with particular concerns with the low energy dependence of $S(E)$ [26].

Haubold and colleagues have reported analytical techniques for the evaluation of Maxwellian averaged nuclear reaction rate coefficients [27–29]. Some additional generalizations and corrections were published by Anderson and Mathai [30] and a review was provided by Mathai and Haubold [31]. The final results for the integrals that arise are in terms of complicated functions whose numerical evaluation is not efficient. This work is primarily of mathematical interest and has not been shown to be a practical method for the efficient calculation of the temperature dependence of nuclear reaction rate coefficients as required in astrophysical applications.

The objective of this paper is to report an efficient analytical representation of the temperature dependence of the nuclear rate coefficients from published nonresonant cross section data for which the astrophysical factor, $S(E)$, can be expressed as a lower order polynomial in the relative energy, E. The method is based on an extension of the well known first order Gaussian approximation to the integrand of the Maxwellian average of the reactive cross section [32] as discussed in Section 2. The asymptotic representation of the higher order moments of the weight function, $w(x) = \exp(-x - b/\sqrt{x})$, $x = E/k_BT$, are used for the analytic representation of the temperature dependence of the rate coefficient where $b = B/\sqrt{k_BT}$, B is the Gamow factor and k_B is the Boltzmann constant. The temperature dependence of the rate coefficient is thus given as a power series in $1/\tau$ or equivalently $T^{\frac{1}{3}}$ where $\tau = 3(b/2)^{\frac{2}{3}}$; see Eq. (8) in Section 2. Although this representation of the rate coefficient has been discussed previously [3,11,20], the coefficients are generally determined with a least squares fitting procedure. In this paper, the coefficients in Eq. (9) are determined analytically with MAPLE to high order and the representation of the rate coefficients is essentially exact. This method is applicable to all nonresonant nuclear reactions for which $S(E)$ is a power series in E [33,34].

With the asymptotic evaluation of the integrals, $\int_0^\infty w(x)x^n\mathrm{d}x$, expressed in terms of τ, a very accurate analytic expression for the temperature dependence of the reactive rate coefficients is obtained. A detailed comparison is made of this representation of the rate coefficients with published results for several typical nuclear reactions, namely D(d, p)T, D(d, n)^{3}He and ^{7}Li(p, α)α. The details of the derivation of the analytic representation of $k(T)$ is discussed in Section 2, the numerical results and comparisons are in Section 3, and a summary is provided in Section 4. In Appendix A, the expressions for $k(T)$ versus T as reported by other researchers are listed for easy comparison with the results reported in this paper. Appendix B is a listing of a MAPLE code used in this work.

2. Analytic representation of the temperature dependence of thermal nonresonant nuclear rate coefficients

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,

$$k(T) = \sqrt{\frac{8}{\pi\mu_g}}\frac{1}{(k_BT)^{3/2}}\int_0^\infty E\mathrm{e}^{-E/k_BT}\sigma(E)\mathrm{d}E \tag{1}$$

where $\mu_g = m_1m_2/(m_1+m_2)$ is the reduced mass in grams and $k(T)$ is in units of $\mathrm{cm}^3\mathrm{mol}^{-1}\mathrm{s}^{-1}$. The reactive cross sections are often written in terms of the astrophysical factor, $S(E)$, and the cross section is given by

$$\sigma(E) = \frac{S(E)}{E}\mathrm{e}^{-B/\sqrt{E}}, \tag{2}$$

where $B = 31.29106Z_1Z_2\sqrt{\mu_a}$ in $\sqrt{\mathrm{keV}}$ is the Gamow factor [32], Z_1 and Z_2 denote the nuclear charges of the two nuclei and μ_a is the reduced mass in atomic mass units (amu) of the reacting nuclei [5,32]. There are numerous analytical representations of the energy dependence of $S(E)$ for different nuclear reactions [2,3,7,35]. For nonresonant reactions, the astrophysical factor can be represented as a power series in the relative energy, E, that is,

$$S(E) = \sum_{n=0}^{N} s_nE^n. \tag{3}$$

With the substitution of Eq. (3) into Eq. (1), the rate coefficient can be written as

$$k(T) = \sqrt{\left(\frac{8}{\pi\mu_gk_BT}\right)}\sum_{n=0}^{N} s_n(k_BT)^nI_n(b). \tag{4}$$