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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

Technical Report 32-1372

Numerical Calculation of Electron-Atom Excitation and Ionization Rates Using Gryzinski Cross Sections

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Preface

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Abstract

Electron-atom excitation and ionization rates were numerically calculated using Gryzinski classical cross sections and Maxwellian electron distributions. A simple analytical expression was obtained which represents the calculations within $\pm 5\%$ over the physically most important range of electron temperatures and atomic parameters. Transition rates calculated from a linear approximation to the cross sections is in poorer agreement with the exact values than this analytical expression.

Numerical Calculation of Electron-Atom Excitation and Ionization Rates Using Gryzinski Cross Sections

I. Introduction

In problems involving ionized gases, it is often of interest to know the electron-atom excitation and de-excitation rates for transitions between specific energy levels of the atoms. Knowledge of such rates is important, for example, in understanding the details of the kinetics of ionization, recombination, and radiative processes in gases.

The excitation rate $K(p,q)$ for transitions from level p to level q is given (Ref. 1) by:

$$K(p,q) = \frac{1}{N_e} \int_{U(p,q)}^{\infty} \frac{dN_e(E)}{dE} v_e(E)\, Q_{p,q}(E)\, dE \qquad (1)$$

where

N_e = the total electron density

$dN_e(E)/dE$ = the electron distribution function in terms of the energy E

$v_e(E) = \left(\frac{2E}{m}\right)^{1/2}$ = the electron velocity

$Q_{p,q}(E)$ = the energy-dependent electron-atom inelastic cross section

$U(p,q)$ = the energy difference between the two levels

This report presents results of the numerical calculation of these transition rates for a wide range of atomic parameters. A Maxwellian distribution was taken for $v_e(E)$. This should be satisfactory for many cases of interest; however, this assumption should be justified for any particular case being considered. Other distribution functions could be used when they are applicable. The Gryzinski (Ref. 2) classical cross sections were used for $Q_{p,q}(E)$ because of their simplicity of calculation and their apparent relatively good agreement with experiment. These classical cross sections are currently quite commonly used for these reasons by many authors (Ref. 3) in spite of their somewhat questionable theoretical justification.[1]

The numerical result have been correlated with a simple analytical expression. This formula can be used to calculate quickly the transition rates within a physically most important range of atomic parameters. It is also shown that this expression predicts the transition rates more accurately than an expression obtained by assuming the cross sections to be linear functions of the energy.

[1] It should be noted that errors in equations presented in Ref. 2 are corrected in Bauer, E., and Bartky, C. D., "Calculation of Inelastic Electron-Molecule Cross Sections by Classical Methods," *J. Chem. Phys.*, *43*, 2466, 1965.

II. Exact Calculation

The Gryzinski cross sections are given by[2]:

$$Q_{p,q}(E) = Q\left(\frac{U_p^i}{U_{p,q}}; \frac{E}{U_{p,q}}\right) - Q\left(\frac{U_p^i}{U_{p,q+1}}; \frac{E}{U_{p,q+1}}\right) \tag{2}$$

$$Q\left(\frac{U_p^i}{U_{p,q}}; \frac{E}{U_{p,q}}\right) = \frac{\sigma_0}{U_{p,q}^2} g_Q \tag{3}$$

$$g_Q = \left[\frac{U_p^{i2} E}{(U_p^i + E)^3}\right]^{1/2} \left\{\frac{U_{p,q}}{U_p^i} + \frac{2}{3}\left[1 - \frac{U_{p,q}}{2E}\right] \times \ln\left[e + \left(\frac{E - U_{p,q}}{U_p^i}\right)^{1/2}\right]\right\} \times \left[1 - \frac{U_{p,q}}{E}\right]^{1 + \frac{U_p^i}{U_p^i + U_{p,q}}} \tag{4}$$

where

$U_p^i =$ the binding energy of level p

$\sigma_0 = 6.56 \times 10^{-14}$ cm^2 (eV)^2.

In Eq. (4), substitution of $\epsilon = E/U_{p,q}$, $A = U_p^i/U_{p,q}$ results in

$$g_Q = \left(\frac{\epsilon}{A + \epsilon}\right)^{3/2} \left\{\frac{1}{\epsilon} + \frac{1}{3}\frac{A}{\epsilon^2}(2\epsilon - 1) \times \ln\left[e + \left(\frac{\epsilon - 1}{A}\right)^{1/2}\right]\right\} \left[1 - \frac{1}{\epsilon}\right]^{\frac{2A+1}{A+1}} \tag{5}$$

The desired transition rate then consists of the difference of two integrals over expressions having the form of Eq. (5). This can be written as

$$K(p,q) = \bar{K}(p,q) - \bar{K}(p,q+1) \tag{6}$$

where each $\bar{K}$ is calculated from the corresponding Eq. (3). Then, each integral can be considered separately. In cases where the q and $(q+1)$ levels are widely separated, the integral involving the latter can be neglected.

[2]For a discussion of Gryzinski's theory see the recent review by Moiseiwitsch, B. L., and Smith, S. J., "Electron Impact Excitation of Atoms," *Rev. Mod. Phys.*, *40*, 238, 1968.

For a Maxwellian distribution at temperature T

$$\bar{K}(p,q) = \left(\frac{8}{m\pi}\right)^{1/2} \frac{y^{3/2}}{U_{p,q}^{3/2}} \sigma_0 \int_1^\infty e^{-\epsilon y} \left(\frac{\epsilon}{A + \epsilon}\right)^{3/2} \left\{1 + \frac{1}{3}\frac{A}{\epsilon} \times (2\epsilon - 1) \ln\left[e + \left(\frac{\epsilon - 1}{A}\right)^{1/2}\right]\right\} \times \left[1 - \frac{1}{\epsilon}\right]^{\frac{2A+1}{A+1}} d\epsilon \tag{7}$$

where $y = U_{p,q}/kT$. It should be noted that $\bar{K}(p,q) \cdot U_{p,q}^{3/2}$ depends only on two "universal" parameters A and y. Hence, numerical evaluation of Eq. (7) for a suitable range of values of these parameters can be applied to any atom of interest.

For example, in potassium, $A = 3$, 4, and 5, respectively, for $4s - 4p$, $5p - 6s$, and $4d - 6p$. In argon, $A = 1.4$, 3, and 6.5, for $3p - 4s$, $4s - 4p$, and $5p - 4d$, respectively. For any lower level p, as the upper level q gets higher $A \to 1$. If $kT = 0.1$ eV, $y = 16$, 3.4, and 2, respectively, for the above transitions in potassium. Similarly, $y = 23$, 3, and 5, respectively, for the above transitions in argon if $kT = 0.5$ eV.

Values of $R = \bar{K}(p,q)\, U_{p,q}^{3/2}$ (in units of cm^3 s^{-1} (eV)$^{3/2}$) were numerically calculated on a computer for $A = 1$, 2, 4, 6, 8, and 10 over a range of $y = 0.01$ to 10. Figure 1 shows the results plotted against y, with A as a parameter. Values of R for small y are plotted with expanded scales in Figs. 2 and 3. It should be noted that, for small enough y (high enough temperature), the transition rate decreases with increasing temperature. This corresponds to the peak of the Maxwellian distribution occurring at an energy higher than the peak of the cross section.

The reason for the curves crossing is that, for small ϵ, which would be important for low temperature, g_Q is larger as A gets smaller. For large enough ϵ (important for high temperature), larger A gives larger g_Q. Thus, for large y, the integral in Eq. (7) is larger for smaller A and, for small enough y, the integral increases with A.

III. Analytic Approximation

By judicious manipulation of these numerical results it is found that to a very good approximation

$$R = \frac{3.84 \times 10^{-6}\, y^t e^{-y}}{A^{1/4}(y^2 + 7y/4 + 1/9)} \tag{8}$$

$$t = \frac{A + 30}{5(2A + 5)}$$

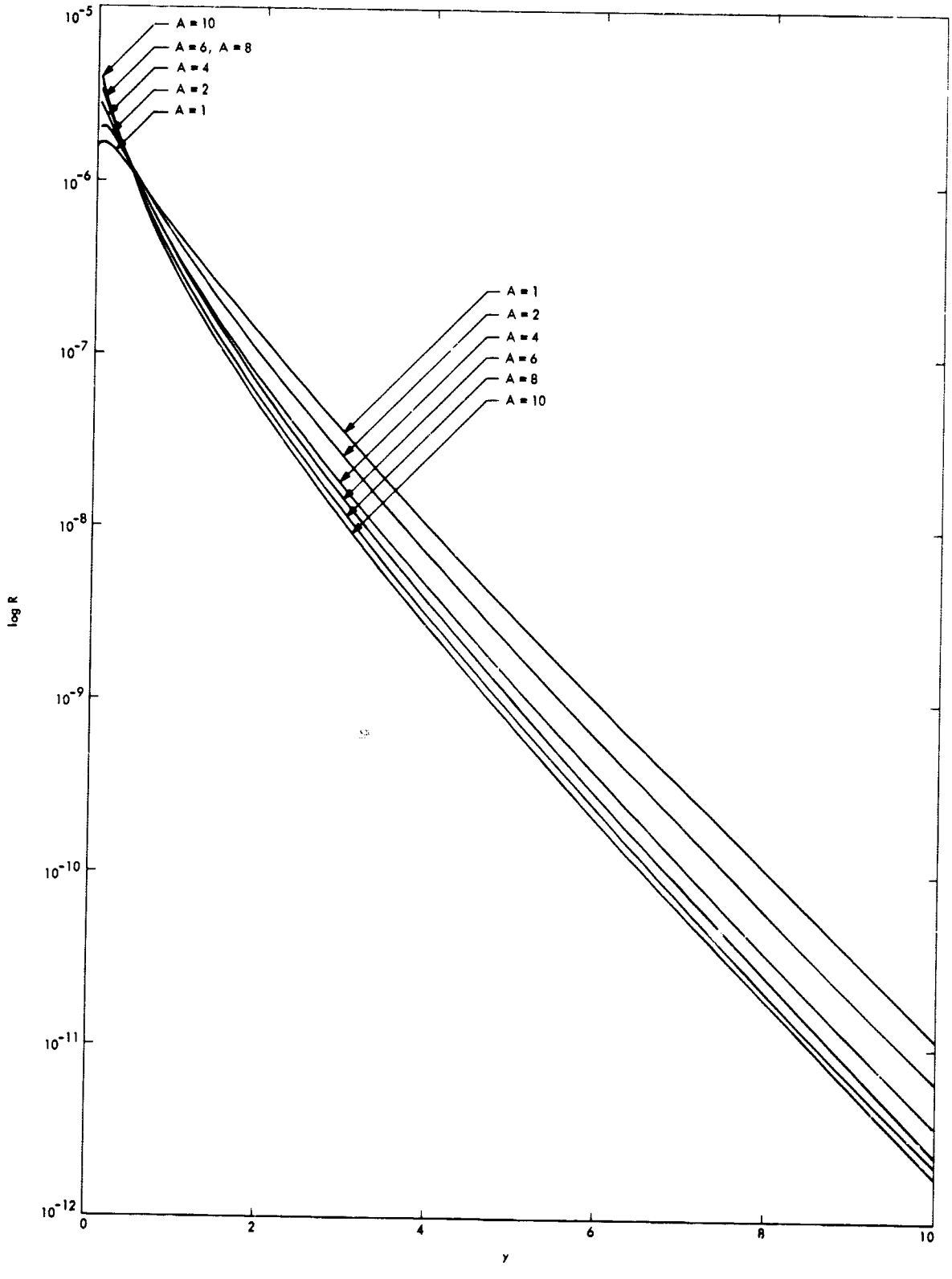

Fig. 1. Calculated excitation rate dependence on parameter $y = U_{p,q}/kT$

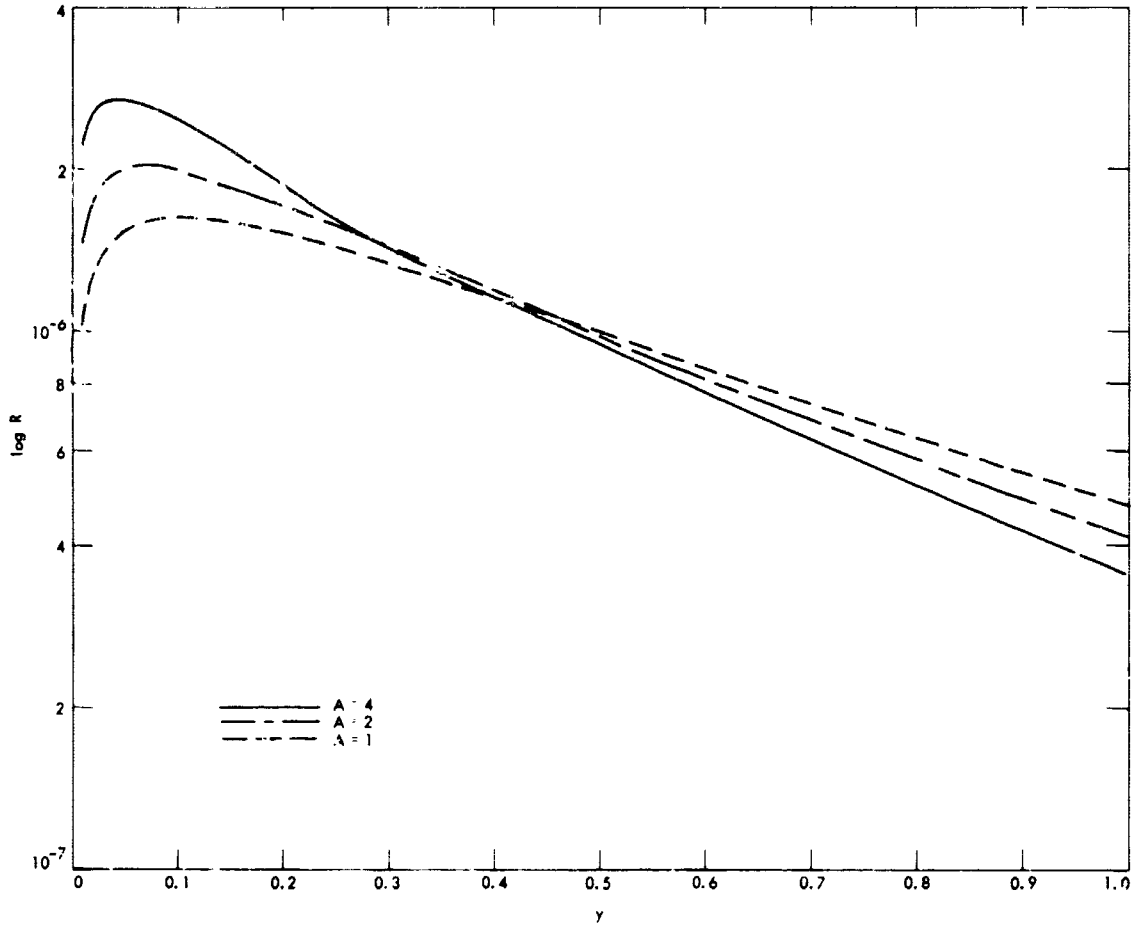

Fig. 2. Calculated excitation rate dependence on parameter $y = U_{p,q}/kT$, high-temperature behavior ($A = 1, 2, 4$)

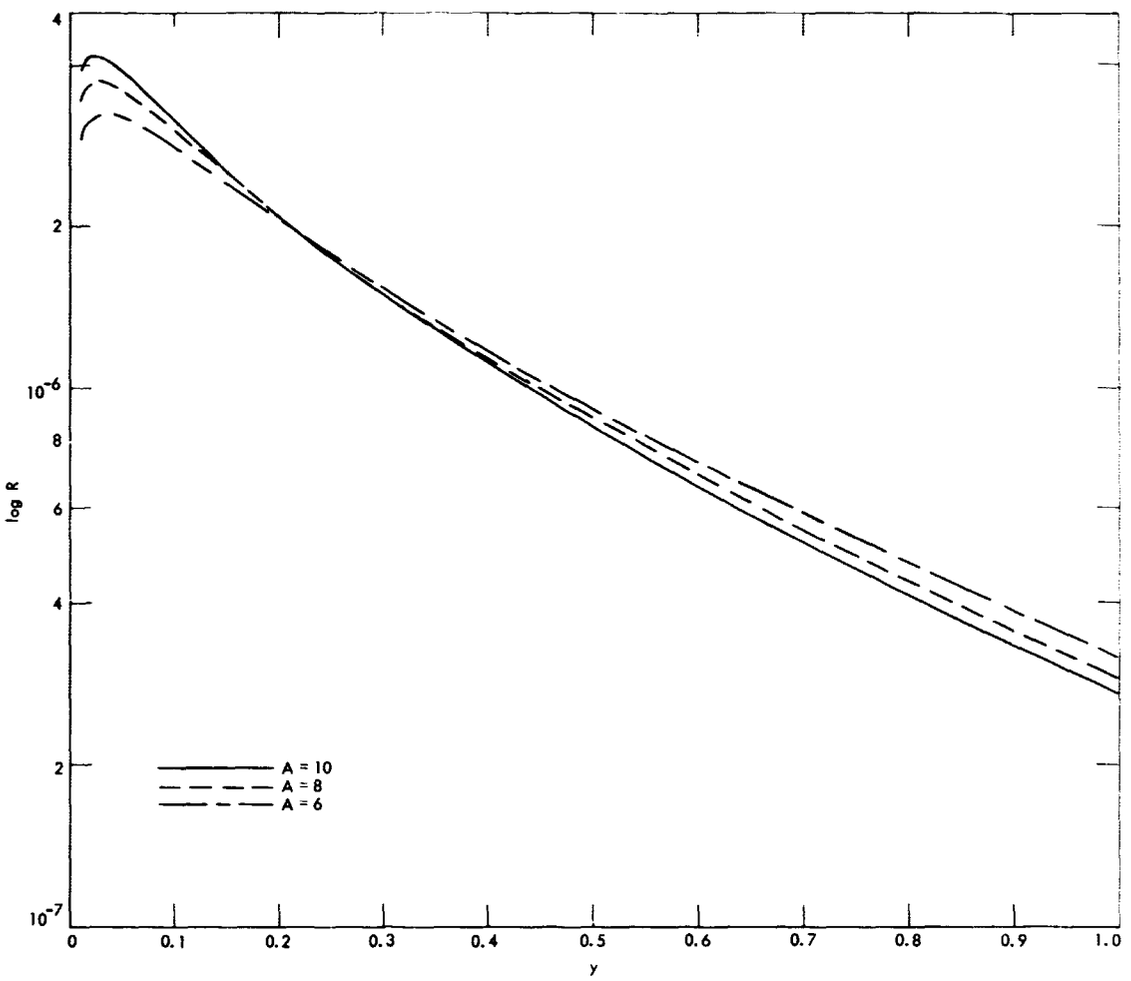

Fig. 3. Calculated excitation rate dependence on parameter $y = U_{p,q}/kT$, high-temperature behavior ($A = 6, 8, 10$)

For $1 \leq A \leq 10$, $0.1 \leq y \leq 10$, this equation reproduces the numerical results to about $\pm 5\%$ or better. For $A > 2$ the equation can be extended down to $y = 0.05$ with similar error. At $y = 0.05$, $A = 1$ the error is less than 20%. Therefore, the rates for the physically most important cases can be conveniently calculated by use of Eqs. (8) and (6).

If $U_{p,q}$ is replaced by U_p^i in the above equations (so that $A = 1$), an expression is obtained for the ionization rate $K(p,c)$ from level p. In this case Eq. (6) becomes $K(p,c) = \bar{K}(p.c)$.

IV. Linear Approximation

Very often, to simplify numerical calculations, collision cross sections are taken to be linear over the energy range of interest. For example, as an approximation to the Gryzinski expression Eq. (4), Byron, et al. (Ref. 4), have taken

$$g_Q' = B(\epsilon - 1) \tag{9}$$

where B is given as a numerical function of A. Use of Eq. (9) instead of Eq. (5) in the integral over the velocity distribution gives

$$R' = \left(\frac{8}{\pi m}\right)^{1/2} \frac{\sigma_0 B}{y^{1/2}} \left[1 + \frac{2}{y}\right] e^{-y} \tag{10}$$

The results of numerical calculations using Eq. (10) are shown in comparison with the exact results in Fig. 4. The ratio R'/R of the linear to exact transition rate is shown as a function of y for three of the values of A under consideration here. Byron states that the linear approximation to the cross section is within 30% of the Gryzinski value if $0.01A \leq y \leq 1 + 0.1A$. Figure 1 shows that these bounds give an error larger than 30% in the integrated transition rate.

The shape of the curves in Fig. 4 can be understood by consideration of the shapes of the Maxwellian tail and the g_Q function. For a given A, the linear approximation will be best when the Maxwellian tail crosses the linear region of g_Q. As y increases (kT decreases) the important

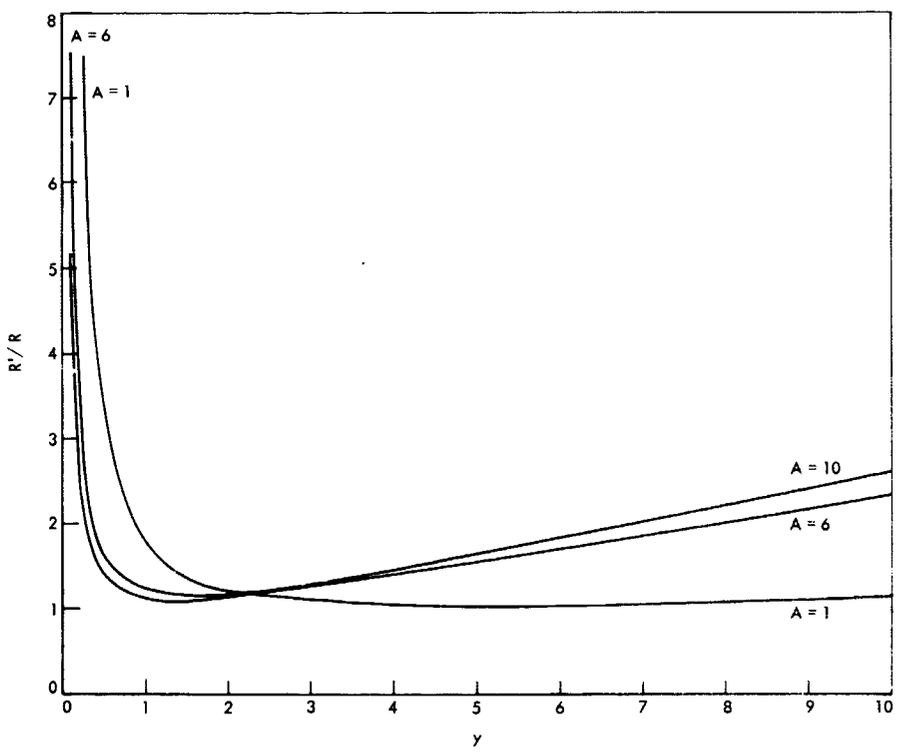

Fig. 4. Ratio of transition rate calculated with linear approximation to that calculated by exact cross section

part of g_Q is the threshold region, which is concave upward. Byron's approximation overestimates the value of g_Q in this region and, hence, also the value of R. For small y (high temperature), contributions come from the region where g_Q is concave downward, so that the linear approximation again overestimates the integral in Eq. (1). As A increases, g_Q becomes flatter and the linear approximation (at least over some range of y) is better.

V. Conclusions

A simple analytical expression has been obtained which represents within $\pm 5\%$ the results of the exact calculation over most of the range of parameters considered. Transition rates calculated from a linear approximation to the cross sections is in poorer agreement with the exact values than this analytical expression.

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