Brief Reports

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Thermally averaged collision strengths for Sr^+

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We use the Gauss-Laguerre method to perform Maxwell averaging of distorted-wave collision strengths for transitions among the lowest three terms of singly ionized strontium. Rate coefficients are readily derived from the thermally averaged collision strengths Υ. By suitably scaling Υ, we form reduced collision strengths $\Upsilon_{\rm red}$ that are finite at all temperatures. Each $\Upsilon_{\rm red}$ is plotted as a function of reduced temperature $T_{\rm red}$, which maps the entire range of T onto the interval [0,1]. We use the least-squares method to fit $\Upsilon_{\rm red}$ by a five-point cubic spline. This fitting procedure has an rms error of less than 1% and is performed on a microcomputer by an interactive program with graphic display.

I. INTRODUCTION

The overabundance of strontium in the outer layers of magnetic Ap stars is believed to be caused by the net outward diffusion of this element.[1] Young main sequence stars with surface temperatures of about 10 000 °K are classified as A-type stars. Those having anomalously intense or variable spectrum lines from elements such as Si, Cr, Mn, Sr, Eu, etc. form a subclass Ap, the subscript signifying peculiar. In order to make a quantitative analysis of the radiative forces that drive the element outwards, one needs to know the level populations of Sr,Sr^+, ... high in the stellar atmosphere. Realistic level populations are provided by non-local-thermodynamic-equilibrium (LTE) calculations in which good quality atomic data are used.

In this paper we compute temperature-dependent collision strengths for transitions induced by thermal electrons between the $5\,^2S$, $4\,^2D$, and $5\,^2P$ levels of Sr^+. These are obtained by Maxwell averaging the energy-dependent distorted-wave collision strengths of Chidichimo.[2] We make use of a new spline-fitting procedure[3] which is a convenient way of interpolating and extrapolating both Ω and Υ.

Our results for the optically allowed transitions ($5s$-$5p$ and $4d$-$5p$) are compared with earlier estimates[1] based on Burgess's semiclassical impact-parameter approximation.[4,5] In addition we give results for the optically forbidden transition ($5s$-$4d$) which until now has been treated very approximately.[1,6]

II. DEFINITIONS

Thermalized free electrons in a stellar atmosphere with kinetic temperature T have a Maxwellian velocity distribution $f(v)$ given by

$$f(v)=(2/\pi)^{1/2}(m_e/kT)^{3/2}v^2\exp(m_e v^2/2kT)\ , \qquad (1)$$

where the symbols have their usual meanings. The collision rate for the transition $i\rightarrow j$ is given by $N_e q(i\rightarrow j)$, where N_e is the electron number density and

$$q(i\rightarrow j)=\int_{(2m_eE_{ij})^{1/2}}^{\infty} Q(i\rightarrow j)v_i f(v_i)dv_i \qquad (2)$$

is the inelastic rate coefficient. $Q(i\rightarrow j)$ is the excitation cross section and E_{ij} is the transition energy. The collision strength Ω is related to Q through

$$Q(i\rightarrow j)=\pi\Omega(i,j)/(g_i k_i^2)\ , \qquad (3)$$

where k_i is the wave number of a free-electron incident on a target ion in level i. To be consistent with Ref. 1 we omit the spin factor $(2S_i+1)=2$ from the definition of the statistical weight g_i. From (3) it can be seen that Ω is a dimensionless quantity; furthermore it is symmetrical in i and j. We rewrite (2) as follows:

$$q(i\rightarrow j)=2.1716\times10^{-8}(I_{\mathrm{H}}/kT)^{1/2}\times\exp(-E_{ij}/kT)\Upsilon(i,j)/g_i\ \mathrm{cm^3\,s^{-1}}\ , \quad (4)$$

where I_{H} is the Rydberg energy (13.60 eV) and

$$\Upsilon(i,j)=\int_0^\infty \Omega(i,j)\exp(-E_j/kT)d(E_j/kT) \quad (5)$$

is the thermally averaged collision strength. Note that $E_j=E_i-E_{ij}$ is the free-electron energy after excitation. The deexcitation rate coefficient $q(j\rightarrow i)$ is given by

$$q(j\rightarrow i)=(g_i/g_j)\exp(E_{ij}/kT)q(i\rightarrow j)\ . \quad (6)$$

III. MAXWELL AVERAGING

We evaluate the integral in (5) using a 15-point Gauss-Laguerre formula.[7] Energy-dependent collision strengths for the rubidiumlike ion Sr^+ are taken from the work of Chidichimo[2] who used a nonexchange Coulomb distorted-wave approximation (CDW II) to compute $\Omega(5s,5p)$, $\Omega(4d,5p)$, and $\Omega(5s,4d)$. We interpolate her data using the program OMEUPS that incorporates the spline-fitting procedure of Burgess and Tully.[3] The program, which is described briefly in Sec. IV, also carries out the Gauss-Laguerre integration and compacts the resulting data by means of a five-point spline.

IV. SPLINE FITTING THE DATA

Burgess and Tully[3] have developed a new method to assess and compact collision strength data for electron-impact excitation of positive ions. The method allows one to (a) interpolate and extrapolate data in energy and temperature; (b) store data in compact form without losing significant information; (c) perform Maxwell averaging; and (d) detect printing and computational errors in tabulated data.

OMEUPS is an interactive graphics program based on this method and was written by A. Burgess. The language used is BBC BASIC and the program runs best on the Archimedes System (ACORN's microcomputer with a RISC microprocessor). By using the emulator BBC BASIC(86) from M-TEK Computer Services, the program can also be run on any IBM or IBM-compatible microcomputer with graphics. OMEUPS has two branches labeled OMEGA and UPSILON. As the names suggest, OMEGA is used for analyzing energy-dependent collision strengths while UPSILON is used for dealing with their thermally averaged counterparts.

The originality of the method hinges on the use of scaling techniques which (i) remove the main energy or temperature dependence from the data and (ii) map the entire range of E or T onto the interval [0,1]. We denote the scaled or reduced variables by E_{red}, Ω_{red} and T_{red}, Υ_{red}.

In OMEGA we let $x=E_{\mathrm{red}}$, $y=\Omega_{\mathrm{red}}$. Then for an optically allowed transition which we denote as type 1,

$$x=1-\ln(C)/\ln(E_j/E_{ij}+C)\ ,\qquad y=\Omega/\ln(E_j/E_{ij}+e)\ , \quad (7)$$

where $C>1$ and $e=2.178\ldots$. For an optically forbidden transition which we denote as type 2,

$$x=(E_j/E_{ij})/(E_j/E_{ij}+C),\quad y=\Omega \quad (8)$$

where $C>0$.

In UPSILON we let $x=T_{\mathrm{red}}$, $y=\Upsilon_{\mathrm{red}}$. For a type-1 transition

$$x=1-\ln(C)/\ln(kT/E_{ij}+C)\ ,\qquad y=\Upsilon/\ln(kT/E_{ij}+e)\ , \quad (9)$$

where $C>1$ and $e=2.718\ldots$. For a type-2 transition

$$x=(kT/E_{ij})/(kT/E_{ij}+C),\quad y=\Upsilon \quad (10)$$

where

$$C>0\ .$$

The parameter C depends on the transition; its value can be adjusted in order to optimize the plot of y versus x prior to making a spline fit.

After inputting the data in the OMEGA branch and providing an initial estimate for C, the collision strength is scaled and displayed as a function of E_{red}. By modifying the value of C one can change the distribution of data points on the plot. The program then uses a five-point least-squares spline to fit the scaled data and draws the corresponding curve on the screen. The spline function $y_s(x)$ for Ω_{red}(CDW II) is tabulated at the five equidistant reduced energy knots ($x\equiv E_{\mathrm{red}}=0.0, 0.25, 0.50, 0.75, 1.0$) in Ref. 2 for the 3 transitions under study. The original data can in this way be readily interpolated or extrapolated, and the program does this in order to carry out the Maxwell averaging outlined in Sec. III. The user specifies the number of temperatures for which Υ is to be calculated. The temperature values are selected automatically in order to divide the entire range of T_{red} into approximately equal intervals. The data so obtained is then scaled and splined in the UPSILON branch of the program. Values of y_s for Υ_{red}(CDW II) at the five mesh points are given in Table I. In all cases the rms error is seen to be less than 1%. The spline function $y_s(x)$ which allows one to interpolate $y(x)\equiv\Omega_{\mathrm{red}}$ or Υ_{red}, using the values of

TABLE I. Values of the spline function $y_s(x)$ for Υ_{red}(CDW II) at the five reduced temperature knots. The parameter C is chosen to minimize the rms error of each fit.

Transition	C	$y_s(0)$	$y_s(\frac{1}{4})$	$y_s(\frac{1}{2})$	$y_s(\frac{3}{4})$	$y_s(1)$	rms error
$5s\rightarrow5p$	5.5	8.391	15.61	19.42	22.72	22.61	0.51%
$4d\rightarrow5p$	8.0	33.19	28.29	28.30	26.39	23.76	0.45%
$5s\rightarrow4d$	6.0	3.56	5.23	5.47	5.56	5.09	0.79%

TABLE II. Thermally averaged collision strengths $\Upsilon(i,j)$. Comparison of SCIP and quantal CDW II approximations at $T=10\,000$ K. The values of r_0 in a.u., E_{ij} in Ry, and f_{ij} are those used in this work.

i,j	SCIP[a]	SCIP[b]	CDW II	r_0	E_{ij}	f_{ij}
$5s,5p$	6.75	10.07	11.48	3.700	0.220 97	1.050
$4d,5p$	5.61	51.16	39.43	2.934	0.086 80	0.0976

[a]Reference 1.
[b]Present results.

$y_s(0)$, $y_s(0.25)$, $y_s(0.5)$, $y_s(0.75)$, $y_s(1)$, and C, is given in Appendix C of Ref. 8 in the convenient form of a short computer program.

V. HIGH-ENERGY AND TEMPERATURE LIMITS

These are often treated cavalierly in extrapolation procedures. For the nonrelativistic approximations which we are using, the values of $y(1)$ can be calculated by fairly simple quantum-mechanical approximations. The definitions of reduced variables lead to the following.

Type 1

$$y(1)=4g_i f_{ij}/(E_{ij}/I_{\mathrm{H}}) \quad \text{for } y=\Omega_{\mathrm{red}} \text{ or } \Upsilon_{\mathrm{red}} . \tag{11}$$

Type 2

$$y(1)=\lim_{E_j/E_{ij}\to\infty} \Omega(i,j) \quad \text{for } y=\Omega_{\mathrm{red}} \text{ or } \Upsilon_{\mathrm{red}} . \tag{12}$$

Note that f_{ij} is the absorption oscillator strength and I_{H} is the Rydberg energy (13.60 eV). The limiting value for a type-2 transition is given by the Born approximation; see, for example, Ref. 9. For the $5s$-$4d$ transition we estimate this to be 4.88.

VI. SEMICLASSICAL APPROXIMATION

Borsenberger *et al.*[1] have used a semiclassical impact-parameter (SCIP) approximation for six allowed transitions in Sr^+. We assume that they thermally averaged these to get values of Υ_{ij}/g_j at $T=10\,000$ K, and that they use the symbol Ω instead of Υ in their Table I. The comparison we make in Table II shows that there are important differences between the SCIP results of Ref. 1 and the quantal calculations. Because of the large discrepancy for the $4d$-$5p$ transition, where $\Upsilon(\text{CDW II})/\Upsilon(\text{SCIP}^a)\sim 7$, we decided to repeat the SCIP calculations. Our results, which are given in Table II under the heading SCIP[b], are seen to be in reasonable agreement (better than a factor of 2) with the CDW II ones.

An important parameter in the SCIP approximation is the radius r_0 of the spherical region occupied by the target ion. We define a length r_{nl} by the hydrogenic formula

$$r_{nl}=(2Z)^{-1}[3\nu^2-l(l+1)] \text{ a.u.} , \tag{13}$$

where Z is the net charge of Sr^{2+} in a.u. and ν is the effective quantum number given by

$$\nu=(Z^2 I_{\mathrm{H}}/|E_{nl}|)^{1/2} . \tag{14}$$

E_{nl} is the energy of the nl term relative to the ground state of Sr^{2+}. We take r_0 to be the smaller of r_{nl} and $r_{n'l'}$ for the transition $nl\to n'l'$. Borsenberger *et al.*[1] may have chosen larger values for r_0 than those shown in Table II and this could explain why their collision strengths are smaller than ours.

We conclude by pointing out the way in which the present SCIP approximation differs from that proposed in Refs. 4 and 5. As is well known, it is physically unrealistic to use the SCIP approximation for close encounters (i.e., penetrating collisions). We therefore exclude the contribution from trajectories with impact parameter $\rho<\rho_0$, where ρ_0 corresponds to an orbit whose closest approach to the nucleus is r_0. Furthermore, following Seaton,[10] we impose the condition that the probability used to define the cross section should not exceed $\frac{1}{2}$. Hence

$$Q_{ij}=\pi(\rho_1^2-\rho_0^2)+2\pi\int_{\rho_1}^{\infty} P_{ij}(\rho)\rho^2 d\rho , \tag{15}$$

where

$$\rho_1=\rho_{1/2} \quad \text{if } \rho_{1/2}>\rho_0 \tag{16}$$

and

$$\rho_1=\rho_0 \text{ if } \rho_{1/2}\le\rho_0 . \tag{17}$$

We have denoted by $\rho_{1/2}$ the value of the impact parameter at which the semiclassical transition probability P_{ij} attains the value $\frac{1}{2}$. This definition for Q is slightly different from that used previously.[4,5] For transitions were strong coupling occurs, the present method yields a smaller estimate for the collision strength at near-threshold energies.

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