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Collisional excitation rates for transitions between the fine structure levels of the ground term of Ne^{2+}

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Summary. A four-state close-coupling approximation is used to obtain electron impact excitation rates for transitions among the levels of the lowest configuration of Ne^{2+}. The results from statistical equilibrium calculations including the new rates show that the intensity ratio $I(15.6\,\mu m)/I(36.0\,\mu m)$ is density sensitive for electron densities in the range of 10^4 to $10^6\,cm^{-3}$ with negligible temperature variation. It is also shown that the ratio $I(15.6\,\mu m)/I(3869\,Å)$ is highly sensitive to temperature for densities less than about $10^5\,cm^{-3}$ with only slight dependence on density. The intensity of the 15.6 μm line is itself a slowly varying function of the physical conditions up to an electron density of about $10^4\,cm^{-3}$ giving the possibility of an accurate determination of the Ne^{2+} abundance when this condition is fulfilled.

1 Introduction

The advent of space-borne infrared observatories enables previously inaccessible regions of the spectrum to be reached. Among possible new data are observations of the fine-structure lines between the levels of the ground terms of several ions of astrophysical importance. These line intensities could be used as accurate density diagnostics because of their insensitivity to temperature. Such spectra will require accurate collision strengths and transition probabilities for their interpretation. We present here calculations for collisional transitions by electron impact among the fine structure levels of the ground term of one of these ions, namely Ne^{2+}. Of these, the $^3P_1$–$^3P_2$ 15.6 μm line has already been detected in planetary nebulae with the IRAS low resolution spectrometer (Pottasch *et al.* 1984), while atmopheric transmission curves given by Traub & Stier (1976) show that it should be possible to observe the $^3P_0$–$^3P_1$ line at 36.0 μm with a suitable detector aboard a balloon platform or a satellite.

A close-coupling expansion is used to describe the Ne^{2+} + electron system in LS-coupling. The intermediate coupling results are then obtained by an algebraic transformation. Since calculations of this sort are discussed elsewhere in the literature, we give only a brief summary of the relevant methods in the next section. The line intensity ratio $I(15.6\,\mu m)/I(36.0\,\mu m)$ is presented in the final section together with the ratio $I(15.6\,\mu m)/I(3869\,Å)$ which is sensitive to temperature because of the large energy difference between the $2p^4\,{}^1D_2$ and ${}^3P_2$ levels of the 3869 Å transition.

2 Collision rates

We have used the Ne^{2+} target wave-functions of Pradhan (1974) who gives further details. However, in the scattering problem we have replaced the calculated term energies with the experimental ones, E_i (Moore 1949). Consequently, we differ from Pradhan regarding the positions of the resonances converging to these energy levels. Integration over the resonances then gives modified values for the collision rates. We give our revised LS-coupling rate coefficients for transitions among the terms of the lowest configuration of Ne^{2+}: $2s^2 2p^4\,{}^3P$, ${}^1D$ and ${}^1S$. They differ from the results of Pradhan by not more than 20 per cent. Our calculations include the terms $2s^2 2p^4\,{}^3P$, ${}^1D$, ${}^1S$ and $2s2p^5\,{}^3P^0$ but we have omitted the $2s2p^5\,{}^1P^0$ term from the present target since resonances converging to this state contribute negligibly at the temperatures of interest ($T_e < 20\,000$ K).

The close-coupling wavefunction for the scattering system has the form

$$\Psi(SL\pi) = \mathcal{A} \sum_{i=1}^{\mathrm{NCHF}} \chi_i \theta_i + \sum_{j=1}^{\mathrm{NCHB}} c_j \Phi_j$$

where χ_i is a target wavefunction, θ_i is a free electron wavefunction, $\mathcal{A}$ is an antisymmetrising operator and the Φ_j are bound channels that compensate for the introduction of orthogonality conditions imposed on the θ_i (Eissner & Seaton 1972). There are NCHF free channels in this expansion of which NCHOP are open. The energy of the scattered electron relative to the term energy E_i (k_i^2) is positive for an open channel while closed channels are those that have $k_i^2 < 0$. The interaction between the closed and open channels gives rise to the resonances in the cross section. The Kohn variational principle for this trial wavefunction Ψ then leads to a set of coupled integrodifferential equations for the θ_i and c_j (Burke & Seaton 1971) that are solved with the program IMPACT (Crees, Seaton & Wilson 1978). A given state of the ion+electron system has total orbital angular momentum quantum number L, total spin S, and parity denoted by π. All contributing $SL\pi$s with $L \leqslant 5$ are included in the calculation and all angular momenta of the scattered electron l, up to and including g waves ($l = 4$).

For an open channel, the normalisation of a particular solution, $\theta_{ii'}$, as $r \to \infty$ is taken to be

$$r\theta_{ii'} \sim k_i^{-1/2}(\sin \zeta_i\, \delta_{ii'} + \cos \zeta_i\, R_{ii'})$$

in which ζ_i is the Coulomb scattering phase at energy k_i^2,

$$\zeta_i = k_i r - \tfrac{1}{2} l_i \pi + (z/k_i) \ln(2k_i r) + \arg \Gamma(l_i + 1 - iz/k_i)$$

for an ionic charge z. This defines the reactance matrix R. From the R matrix, the scattering matrix may be obtained via the relation

$$S = (1 + iR)(1 - iR)^{-1}$$

and the collision strength in LS-coupling through

$$\Omega(i,j) = \tfrac{1}{2} \sum_{SL\pi} (2S+1)(2L+1) \sum_{l_i l_j} |T^{LS}(il_i, jl_j)|^2 \tag{1}$$

Table 1. Effective collision strengths Υ for transitions between the terms of the lowest configuration of Ne^{2+} in LS-coupling.

TEMPERATURE (K)	$\Upsilon(^1D - {}^3P)$	$\Upsilon(^1S - {}^3P)$	$\Upsilon(^1S - {}^1D)$
5000	1.630	0.1514	0.1995
6000	1.640	0.1571	0.2072
7000	1.646	0.1612	0.2131
8000	1.649	0.1643	0.2179
9000	1.650	0.1668	0.2221
10000	1.650	0.1687	0.2258
11000	1.650	0.1704	0.2294
12000	1.649	0.1718	0.2329
13000	1.648	0.1731	0.2364
14000	1.647	0.1742	0.2399
15000	1.646	0.1751	0.2433
16000	1.644	0.1760	0.2467
17000	1.642	0.1769	0.2500
18000	1.640	0.1777	0.2533
19000	1.637	0.1784	0.2565
20000	1.635	0.1791	0.2596

where $\mathrm{T} = 1 - S$ and l_i, l_j are the orbital angular momenta of the scattered electron associated with the target terms $i(=\Gamma_i S_i L_i)$ and $j(=\Gamma_i S_j L_j)$. Γ represents all other quantum numbers needed to define the term. The effective collision strength Υ is defined by

$$\Upsilon(i-j) = \int_0^\infty \Omega(i,j) \exp(-k_i^2/\kappa T_e)\, d(k_i^2/\kappa T_e).$$

Here κ is Boltzmann's constant in ryd K^{-1} and T_e is the electron temperature in K. In Table 1 we tabulate $\Upsilon(i-j)$ for the $^1D-{}^3P$, $^1S-{}^3P$ and $^1S-{}^1D$ transitions in the temperature range, 5000 K–20 000 K. The downward collision rate coefficient is then

$$q(i-j) = \frac{8.631 \times 10^{-6}}{T_e^{1/2}\omega_i} \Upsilon(i-j) \qquad \mathrm{cm^3\ s^{-1}},$$

ω_i being the statistical weight of the upper state. The upward rate is given by detailed balancing arguments to be

$$q(j-i) = \frac{\omega_i}{\omega_j} q(i-j) \exp\{-(E_i - E_j)/\kappa T_e\}.$$

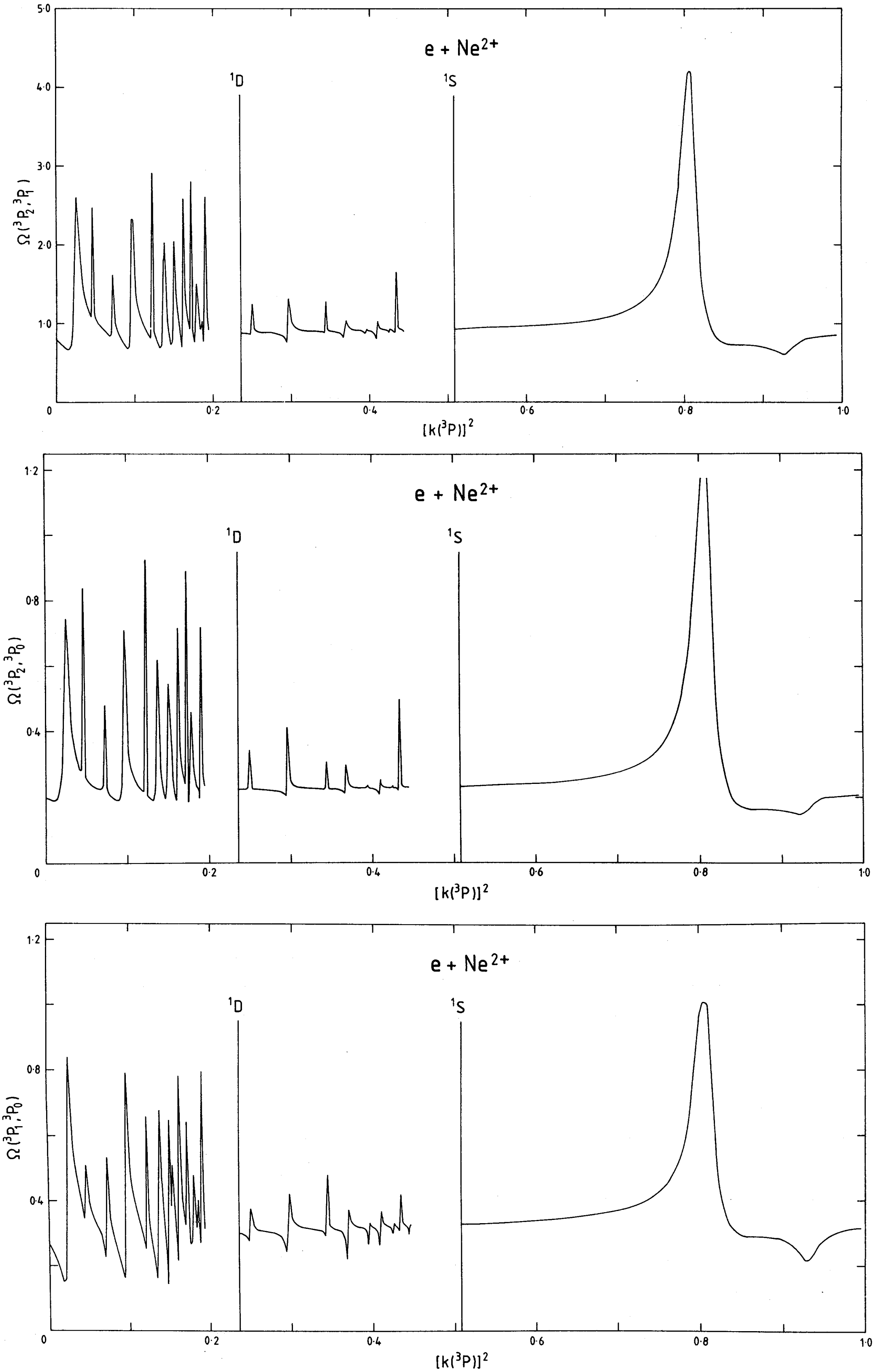

Figure 1. Total collision strengths as a function of scattered electron energy for the fine-structure transitions in the ground term $3s^2\,3p^4\,{}^3$P of Ne^{2+}: (a) $J = 2$ to $J = 1$, (b) $J = 2$ to $J = 0$ and (c) $J = 1$ to $J = 0$.

We have transformed the LS coupling *R* matrices with the program JAJOM (Saraph 1972, 1978). Since we have neglected the perturbations caused by the relativistic part of the interaction, the method is purely algebraic and the *R* matrices in intermediate coupling are easily obtained. Because the fine structure splittings for this ion, and therefore the relativistic effects, are small, the approximation should be a good one. The expression (1) for the collision strength is modified to read

$$\Omega(i,j) = \tfrac{1}{2}\sum_{J\pi}(2J+1)\sum_{l_i l_j} |T^J(il_i, jl_j)|^2.$$

The total angular momentum quantum number is denoted by J and $i = \Gamma_i S_i L_i J_i$ $j = \Gamma_j S_j L_j J_j$ are the levels involved in the transition.

The resultant collision strengths may be seen in Figs. 1a, b and c, for transitions between the $J = 1$ and 2 levels, the $J = 0$ and 2 levels, and the $J = 0$ and 1 levels of the ^{3}P term respectively. Effective collision strengths for these transitions are given in Table 2. They are almost a factor of two larger than the values given by Saraph, Seaton & Shemming (1969) who neglect the resonant contributions altogether.

Table 2. Intermediate coupling effective collision strengths Υ for transitions among the fine structure levels of the $2s^2\,2p^4\,{}^3$P term of Ne^{2+}.

TEMPERATURE (K)	$\Upsilon(^3P_1 - {}^3P_2)$	$\Upsilon(^3P_0 - {}^3P_2)$	$\Upsilon(^3P_0 - {}^3P_1)$
5000	1.089	0.2997	0.3312
6000	1.106	0.3034	0.3380
7000	1.117	0.3055	0.3426
8000	1.125	0.3065	0.3457
9000	1.129	0.3069	0.3479
10000	1.132	0.3068	0.3494
11000	1.134	0.3064	0.3504
12000	1.134	0.3058	0.3510
13000	1.134	0.3049	0.3512
14000	1.133	0.3040	0.3513
15000	1.132	0.3030	0.3512
16000	1.130	0.3020	0.3511
17000	1.129	0.3009	0.3508
18000	1.127	0.2999	0.3504
19000	1.125	0.2987	0.3500
20000	1.122	0.2977	0.3497

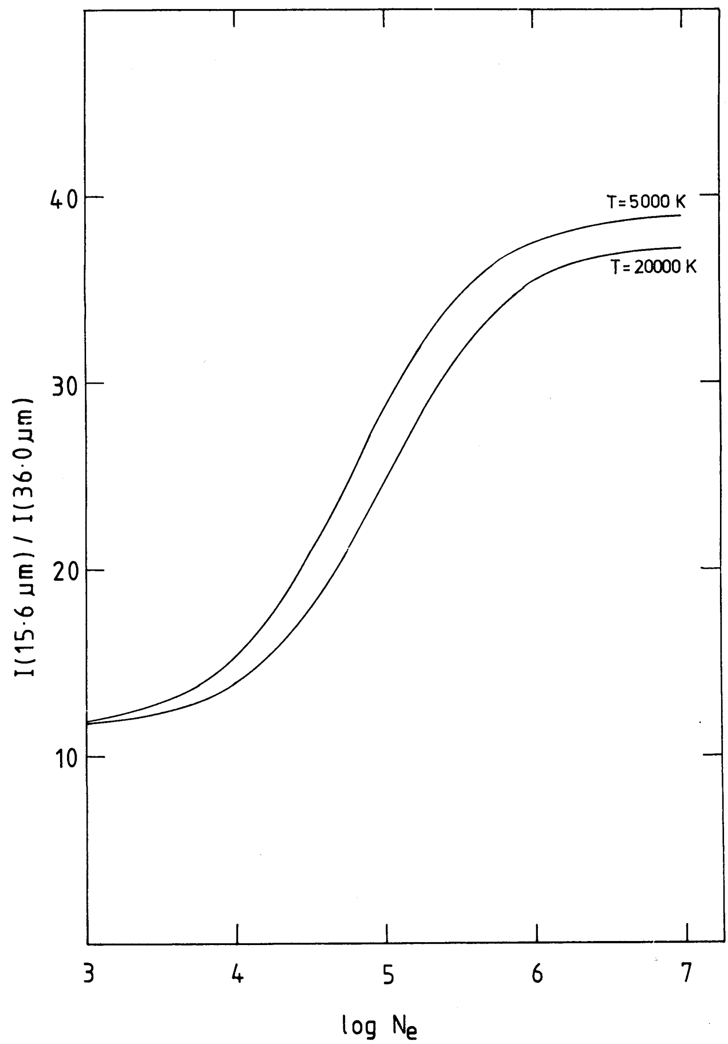

Figure 2. The intensity ratio $I(15.6\ \mu m)/I(36.0\ \mu m)$ plotted as a function of $\log N_e$ at temperatures of 5000 K and 20 000 K.

3 Applications to astrophysical plasmas

We have used these collision rates, together with the transition probabilities of Mendoza & Zeippen (1984, in preparation), as quoted by Mendoza (1983), and the energy levels o Moore (1949) in statistical equilibrium calculations. The plasma was assumed to be opticall thin at the line frequencies and only collisional excitation and de-excitation and spontaneou radiative rates were taken into account. These computations give the line intensity ratio displayed in Fig. 2 and Fig. 3. From Fig. 2 it may be seen that $I(15.6\ \mu m)/I(36.0\ \mu m)$ i density sensitive in the range of electron densities, $N_e \sim 10^4 - 10^6\ \mathrm{cm}^{-3}$ with little tempera ture variation. It should be noted that the $15.6\,\mu m$ line intensity is almost independent o both density and temperature up to densities of about $10^4\ \mathrm{cm}^{-3}$. Within a factor of 1.6 th value of $N(\mathrm{H}) I(15.6\,\mu m)/N(\mathrm{Ne}^{2+}) I(\mathrm{H}\beta)$ is 2×10^4. This line may therefore provide a direc Ne^{2+} abundance determination when the electron density is sufficiently low. Also, the rati $I(15.6\,\mu m)/I(3868.9\ \text{Å})$ varies rapidly with temperature but not with density for densitie $\lesssim 10^5\ \mathrm{cm}^{-3}$, as shown in Fig. 3. Thus observation of the $15.6\,\mu m$ and 36.0-m lines shoul prove a valuable addition to the armoury of those involved in the investigation of this ion i low density astrophysical plasmas.

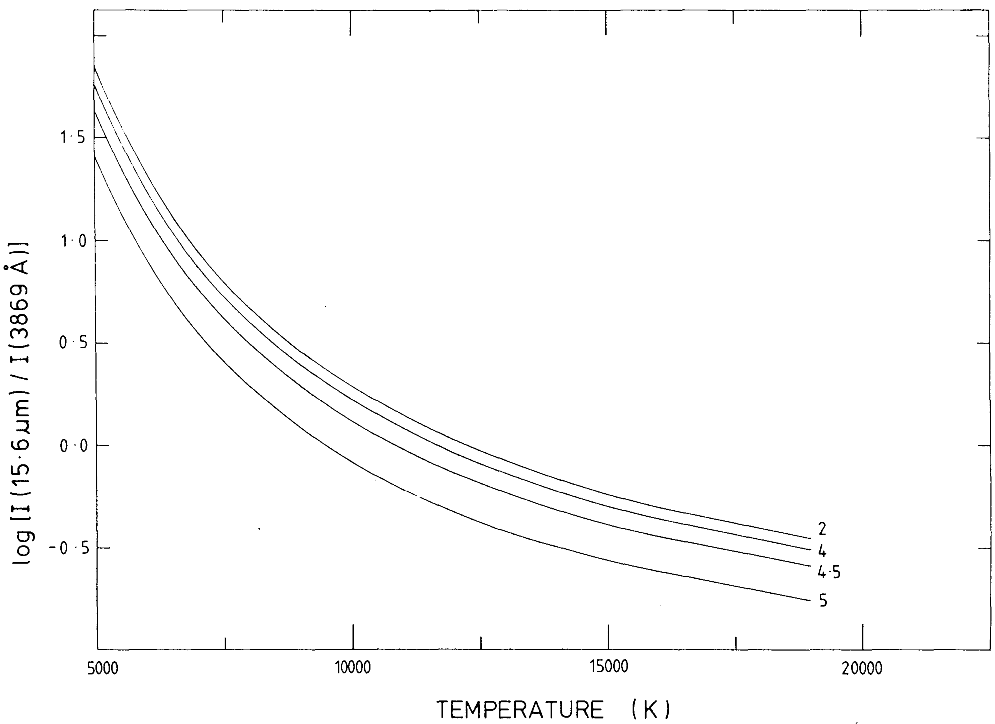

Figure 3. The intensity ratio $I(15.5\ \mu\text{m})/I(3869\ \text{Å})$ as a function of temperature in K. The curves are labelled with the value of $\log N_e$.

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