

Excitation of Forbidden Lines in Gaseous Nebulae I. Formulation and Calculations for $2p \text{ } ^q\text{ } \text{Ions}$

Hannelore E. Saraph, M. J. Seaton and Jillian Shemming

Phil. Trans. R. Soc. Lond. A 1969 **264**, 77-105

doi: 10.1098/rsta.1969.0004

Email alerting service

Receive free email alerts when new articles cite this article - sign up in the box at the top right-hand corner of the article or click [here](#)

To subscribe to *Phil. Trans. R. Soc. Lond. A* go to: <http://rsta.royalsocietypublishing.org/subscriptions>

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE

I. FORMULATION AND CALCULATIONS FOR $2p^q$ IONS

BY HANNELORE E. SARAPH, M. J. SEATON, F.R.S. AND JILLIAN SHEMMING*

*Department of Physics, University College London**(Received 22 May 1968)*

CONTENTS

	PAGE		PAGE
1. INTRODUCTION	78	2.8. The distorted wave approximation	93
2. FORMULATION	80	2.9. Energy variation of collision strengths	93
2.1. General formulation of the collision problem	80	2.10. Discussion of the formulation	94
2.2. Variational principles	81	3. CALCULATIONS	94
2.3. Atomic wave functions	82	3.1. Numerical and computational procedures	94
2.4. Wave functions for the collision problem	87	3.2. Collision strengths in LS coupling	96
2.5. Reduction of integrals	88	3.3. Transitions between fine structure levels	102
2.6. Radial equations	90	REFERENCES	103
2.7. The exact resonance approximation	91		

A formulation is given for electron collisions with ions in configurations $1s^22s^22p^q$ and $1s^22s^22p^63s^23p^q$. The main approximation is neglect of coupling to other configurations. Hartree-Fock functions are used for the ion states and the complete wave functions are expressed as sums of vector-coupled anti-symmetrized products of ion functions and orbitals for the colliding electron. Variational principles are used to obtain coupled integro-differential equations for the radial functions for the colliding electron, and to correct results obtained from approximate solutions of these equations. All algebraic reductions are carried out without the introduction of subsidiary approximations, and conservation and reciprocity theorems are therefore satisfied exactly. Expressions are tabulated for all algebraic coefficients.

Numerical calculations are made in two approximations: in the exact resonance approximation, used only for p -waves, the wave functions are calculated with quadrupole interactions neglected; and in the distorted wave approximation the wave functions are calculated from static central potentials. Variational corrections are calculated and are found to be reasonably small. It is concluded that the final corrected results should agree closely with results which would be obtained from exact solutions of the coupled equations.

Collision strengths are calculated for all inelastic collisions in configurations $1s^22s^22p^q$, $q = 1$ to 5, for at least three different energies, and for values of the residual charge $z = 1, 2, 3, 4, 5$ and the limit of $z \rightarrow \infty$. Results may be interpolated for all members of the iso-electronic sequences. Results for energies such that some channels are open and others closed are obtained by means of extrapolation techniques.

* Now at Norwich City College.

1. INTRODUCTION

The spectra of gaseous nebulae were first observed by W. Huggins and described in a paper published in these *Philosophical Transactions* in 1864. They are characterized by bright emission lines which are due to familiar permitted transitions in hydrogen and helium, and to forbidden transitions in ions of oxygen, nitrogen, sulphur and other elements (Bowen 1928). It was suggested by Bowen that the permitted lines are excited by radiative recombination and that the forbidden lines are excited by electron impact, and the correctness of these ideas has been confirmed by all subsequent work. The present series of papers is concerned with the calculation of excitation rates for the forbidden lines.

The ions which give rise to forbidden lines in the visible spectrum have configurations $2p^q$ and $3p^q$ with $q = 2, 3$ and 4 ; these configurations contain three terms (3P , 1D and 1S for $q = 2$ and 4 and 4S , 2D and 2P for $q = 3$). In many nebulae the strongest lines at $\lambda\lambda 5007, 4959$, are due to the transitions $^1D \rightarrow ^3P_2$ and $^1D \rightarrow ^3P_1$ in the $1s^2 2s^2 2p^2$ configuration of O^{2+} . A weaker line, at $\lambda 4363$, arises from the $O^{2+} \ ^1S \rightarrow ^1D$ transition. For sufficiently low electron densities, collisional deactivation can be neglected and the forbidden line intensities are then proportional to the rates of collisional excitation. In this case, the relative intensities of the lines of a given ion, such as the O^{2+} ratio $I(\lambda\lambda 5007, 4959)/I(\lambda 4363)$, depend only on the electron temperature and from the observed ratios temperatures can be deduced (Ambartsumian 1933; Menzel, Aller & Hebb 1941). At densities which obtain in typical nebulae, it is found that collisional deactivation is important for some of the lines and that certain intensity ratios are sensitive to both electron temperature and electron density. The intensity ratio of the doublet, $\lambda\lambda 3726, 3729$, which results from the transition $^2D \rightarrow ^4S$ in O^+ , provides a particularly useful indication of electron density (Aller, Ufford & Van Vleck 1949; Seaton & Osterbrock 1957). In general, it is possible to deduce both electron temperatures and electron densities from the observed relative intensities of the forbidden lines, and to deduce ion abundances, relative to hydrogen ion abundances, on comparing forbidden line intensities with the intensities of hydrogen lines.

In addition to the forbidden lines in the visible, further forbidden lines will be emitted in the ultraviolet and the infrared parts of the spectrum. The infrared lines, which are of particular importance in connexion with studies of the thermal balance in nebulae, arise from transitions between the fine structure components of the ground terms in ions with configurations np , np^2 , np^4 and np^5 .

The first attempts to calculate the cross-sections for excitation of the forbidden lines were made by Yamanouchi, Inui & Amemiya (1940), who considered O^0 , and by Hebb & Menzel (1940) who considered O^{2+} . Hebb & Menzel expressed the collision cross-section $Q(i \rightarrow j)$ in terms of a dimensionless parameter $\Omega(i, j)$

$$Q(i \rightarrow j) = \frac{\Omega(i, j)}{k_i^2 \omega_i} \pi a_0^2, \quad (1.1)$$

where ω_i is the statistical weight of the initial ion level, $k_i = mv_i/\hbar$ where v_i is the initial velocity of the colliding electron, and a_0 is the Bohr radius. The parameters Ω , which we shall refer to as *collision-strengths*, are symmetrical in initial and final states, $\Omega(i, j) = \Omega(j, i)$. It was shown by Hebb & Menzel that, when account is taken of long-range Coulomb

forces, the collision strengths for positive ions remain finite at excitation thresholds. With a Maxwell distribution of electron velocities the rate coefficient for collisional excitation is

$$q(i \rightarrow j) = \frac{8.63 \times 10^{-6}}{\omega_i T^{\frac{1}{2}}} \int \Omega(i, j) e^{-W_i/kT} d\left(\frac{W_i}{kT}\right) \text{cm}^3 \text{s}^{-1}, \quad (1.2)$$

where $W_i = \frac{1}{2}mv_i^2$ and T ($^{\circ}\text{K}$) is the temperature. If Ω is taken to be a constant this reduces to

$$q(i \rightarrow j) = \frac{8.63 \times 10^{-6}}{\omega_i T^{\frac{1}{2}}} \Omega(i, j) e^{-E_{ij}/kT} \text{cm}^3 \text{s}^{-1}, \quad (1.3)$$

where E_{ij} is the excitation energy.

The work of Yamanouchi *et al.* and of Hebb & Menzel, was discussed in detail by Bates, Fundaminsky & Massey (1950) and criticized on the grounds that the results obtained violated both conservation theorems and reciprocity theorems. The violation of conservation conditions resulted from the assumption of weak coupling between initial and final states, and the use of perturbation theory expressions for the calculation of scattering amplitudes. The violation of reciprocity conditions (the 'post-prior' discrepancy) resulted from an inconsistency in the formulation employed; the expressions for the scattering amplitudes were simplified on making the assumption that exact ion wave functions were to be employed, but approximate ion functions were then substituted into these simplified expressions.

In order to make improved calculations of the forbidden line cross-sections it was necessary to develop better methods of treating electron exchange in collision problems. This was considered by Seaton (1953*a*), who gave a formulation in terms of coupled integro-differential equations. This formulation was such that conservation conditions are satisfied automatically but the difficulty of the post-prior discrepancy was not completely overcome. Calculations were made for O^0 , O^+ , O^{2+} , N^+ , Ne^{2+} and S^+ (Seaton 1953*a, b*, 1955*a, b*, 1958) and approximate estimates were obtained for other ions. These results have been used extensively for the interpretation of nebular spectra. In recent years a great deal of effort has been devoted to making accurate observations of the line intensities in gaseous nebulae (see review article by Aller & Liller 1968) and to making accurate calculations of the radiative transition probabilities (see review article by Garstang 1968).

The present series of papers describes the results obtained in an extensive new programme of calculations of collision cross-sections. Improvements on the earlier work are possible in consequence of advances in atomic collision theory and in the availability of high speed computing facilities. All calculations for ions in $2p^q$ configurations have been made at University College London and similar calculations for ions in $3p^q$ configurations have been made by Dr S. J. Czyzak and Mr T. K. Krueger of the Aerospace Research Laboratories, Wright-Patterson Air Force Base, and Ohio State University.

The formulation employed is discussed in the present paper, and results are given for $2p^q$ ions. Later papers will give results for $3p^q$ ions and results obtained on using methods of quantum defect theory to check the accuracy of the calculations and to make semi-empirical corrections.

Some preliminary accounts of our work have been published previously (Shemming 1965; Saraph *et al.* 1966; Czyzak & Krueger 1967; Czyzak *et al.* 1967, 1968) and more general reviews of collision processes in nebulae have been published by Seaton (1968*a, b*).

2. FORMULATION

2.1. General formulation of the collision problem

We consider electron collisions with an ion containing N electrons and having a nuclear charge Z . We denote the ion wave functions by

$$\Psi(\gamma_i S_i L_i M_{S_i} M_{L_i} | 1, 2, \dots, N), \quad (2.1)$$

where $1, 2, \dots, N$ indicate the space and spin coordinates of the ionic electrons. We use capital Greek letters for wave functions which are completely anti-symmetric. We introduce one-electron orbitals

$$\varphi(l m_s m_l | t) = \chi_{m_s}(\sigma_t) Y_{l m_l}(\hat{\mathbf{r}}_t) (1/r_t) F(r_t) \quad (2.2)$$

where χ_{m_s} is a spin function, $Y_{l m_l}$ a spherical harmonic, and F a radial function, and form the vector-coupled functions

$$\varphi(\gamma_i S_i L_i l S L M_S M_L | t^{-1}; t) = \sum_{M_{S_i} M_{L_i} m_s m_l} C_{M_{S_i} m_s M_S}^{S_i \frac{1}{2} S} C_{M_{L_i} m_l M_L}^{L_i l} \Psi(\gamma_i S_i L_i M_{S_i} M_{L_i} | t^{-1}) \varphi(l m_s m_l | t), \quad (2.3)$$

where t^{-1} is written for the set of coordinates $1, 2, \dots, t-1, t+1, \dots, N+1$. Finally, we form anti-symmetric functions

$$\Phi(1, 2, \dots, N+1) = \frac{(-1)^{N+1}}{\sqrt{(N+1)}} \sum_{t=1}^{N+1} (-1)^t \varphi(t^{-1}; t). \quad (2.4)$$

We use α to indicate the set of quantum numbers $\gamma_i S_i L_i l S L M_S M_L$ and take the wave functions for the entire system to be

$$\Psi_\beta = \sum_\alpha \Phi_\beta(\alpha), \quad (2.5)$$

where β specifies a boundary condition. The radial functions in $\Phi_\beta(\alpha)$ are denoted by $F_{\alpha\beta}$. We take these radial functions to be such that Ψ_β is a solution of the Schrödinger equation,

$$(H - E) \Psi_\beta = 0 \quad (2.6)$$

where

$$H = - \sum_{t=1}^{N+1} \left(\nabla_t^2 + \frac{2Z}{r_t} \right) + \sum_{t'=t+1}^{N+1} \sum_{t=1}^N \frac{2}{r_{tt'}} \quad (2.7)$$

is the Hamiltonian, in rydbergs, for the complete system. The total energy is

$$E = E_\alpha + k_\alpha^2, \quad (2.8)$$

where E_α is the ion energy and k_α^2 the energy of the colliding electron. The radial functions are taken to be zero at the origin and to have asymptotic form

$$F_{\alpha\beta}(r) \sim_{r \rightarrow \infty} k_\alpha^{-\frac{1}{2}} \{ (\sin x_\alpha) C_{\alpha\beta} + (\cos x_\alpha) D_{\alpha\beta} \}, \quad (2.9)$$

where

$$x_\alpha = k_\alpha r - \frac{1}{2} l_\alpha \pi + \frac{z}{k_\alpha} \ln(2k_\alpha r) + \arg \Gamma \left(l_\alpha + 1 - \frac{iz}{k_\alpha} \right) \quad (2.10)$$

and where $z = (Z - N)$ is the residual charge on the ion. When standard phase conventions are adopted, we may take the matrices \mathbf{C} and \mathbf{D} to be real.

The *reactance matrix*, $\mathbf{R} = \mathbf{D}\mathbf{C}^{-1}$, is real and symmetric and is diagonal in $SLM_S M_L$. Further, the elements diagonal in $SLM_S M_L$ are independent of $M_S M_L$. The *scattering matrix* is $\mathbf{S} = (\mathbf{1} + i\mathbf{R})(\mathbf{1} - i\mathbf{R})^{-1}$ and the collision strengths are given by (Seaton 1962)

$$\Omega(\gamma_i S_i L_i, \gamma'_i S'_i L'_i) = \frac{1}{2} \sum_{u' SL} (2S+1)(2L+1) |S(\gamma_i S_i L_i l SL, \gamma'_i S'_i L'_i l' SL)|^2. \quad (2.11)$$

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE 81

To obtain collision strengths for transitions between fine structure states it is convenient to make a transformation to $J_i j$ coupling

$$S(\gamma_i S_i L_i J_i l j J, \gamma'_i S'_i L'_i J'_i l' j' J) = \sum_{SL} A \begin{pmatrix} S_i & L_i & J_i \\ \frac{1}{2} & l & j \\ S & L & J \end{pmatrix} S(\gamma_i S_i L_i l S L, \gamma'_i S'_i L'_i l' S L) A \begin{pmatrix} S'_i & L'_i & J'_i \\ \frac{1}{2} & l' & j' \\ S & L & J \end{pmatrix}, \quad (2.12)$$

$$\Omega(\gamma_i S_i L_i J_i, \gamma'_i S'_i L'_i J'_i) = \frac{1}{2} \sum_{u' j j' J} (2J+1) |S(\gamma_i S_i L_i J_i l j J, \gamma'_i S'_i L'_i J'_i l' j' J)|^2. \quad (2.13)$$

These expressions may be simplified if one of the two terms contains only one fine structure level. Using known properties of the transformation coefficients (Edmonds 1957) we obtain

$$\Omega(\gamma_i S_i L_i, \gamma'_i S'_i L'_i J'_i) = \left. \begin{aligned} & \frac{(2J'_i+1)}{(2S'_i+1)(2L'_i+1)} \Omega(\gamma_i S_i L_i, \gamma'_i S'_i L'_i) \\ & \text{if } S_i = 0 \quad \text{or if } L_i = 0. \end{aligned} \right\} \quad (2.14)$$

2.2. Variational principles

The asymptotic form (2.9) may be written

$$\mathbf{F} \sim k^{-\frac{1}{2}} \{(\sin x) \mathbf{C} + (\cos x) \mathbf{D}\} \quad (2.15)$$

in matrix notation, it being understood that quantities in italic type, without subscripts, are diagonal matrices. Taking

$$\left. \begin{aligned} \mathbf{C} &= \cos \tau - (\sin \tau) \boldsymbol{\rho}, \\ \mathbf{D} &= \sin \tau + (\cos \tau) \boldsymbol{\rho}, \end{aligned} \right\} \quad (2.16)$$

we obtain

$$\mathbf{F} \sim k^{-\frac{1}{2}} \{\sin(x+\tau) + (\cos(x+\tau)) \boldsymbol{\rho}\} \quad (2.17)$$

and

$$\mathbf{R} = [\sin \tau + (\cos \tau) \boldsymbol{\rho}] [\cos \tau - (\sin \tau) \boldsymbol{\rho}]^{-1}. \quad (2.18)$$

Consider functions Ψ'_β containing radial functions $F_{a\beta}$ with asymptotic form (2.17) and functions $(\Psi'_\beta + \delta\Psi'_\beta)$ containing radial functions $(F_{a\beta} + \delta F_{a\beta})$ with asymptotic form

$$\mathbf{F} + \delta\mathbf{F} \sim k^{-\frac{1}{2}} \{\sin(x+\tau) + (\cos(x+\tau)) (\boldsymbol{\rho} + \delta\boldsymbol{\rho})\}, \quad (2.19)$$

where it is to be noted that the diagonal matrix τ is not varied. Defining matrices \mathbf{L} and $\mathbf{L} + \delta\mathbf{L}$ with elements

$$L_{\beta'\beta} = (\Psi'_{\beta'} | H - E | \Psi'_\beta), \quad (2.20)$$

$$L_{\beta'\beta} + \delta L_{\beta'\beta} = (\Psi'_{\beta'} + \delta\Psi'_{\beta'} | H - E | \Psi'_\beta + \delta\Psi'_\beta) \quad (2.21)$$

we obtain the variational principle that, for small variations about the exact functions,

$$\delta\{\boldsymbol{\rho} - \mathbf{L}\} = 0 \quad (2.22)$$

(Kohn 1948).

If the condition (2.22) is satisfied for *all possible* small variations of the functions, consistent with the asymptotic forms (2.17) and (2.19), then these functions must be exact solutions of the Schrödinger equation. In practice we impose certain restrictions on the functions, such as retaining only a finite number of terms in the expansion (2.5). In this case the 'best'

functions may be determined by requiring that (2.22) should be satisfied for all small variations consistent with these restrictions.

A further use of the variational principle is to obtain corrections to the ρ matrix. Suppose that we have approximate functions Ψ^t containing matrices ρ^t . An improved estimate for ρ is

$$\rho^K = \rho^t - L^t. \quad (2.23)$$

The error in ρ^K is of quadratic order in the error in the wave functions.

With $\tau = 0$ we have $\rho = \mathbf{R}$. It sometimes happens that the elements of \mathbf{R} are large. This may be appreciated by considering one-channel cases, for which the phase-shift, $\xi = \arctan R$, may be close to $\frac{1}{2}\pi$. When R is large the variational principle will not give reliable results if τ is taken to be zero. In practice the phases τ are chosen to be such that ρ is not large. The precise choice adopted will be discussed in §2.8.

Some use is also made of a variational principle for the scattering phase matrix,

$$\xi = \arctan \mathbf{R}.$$

Putting $\mathbf{R}\mathbf{X} = \mathbf{X}\bar{\mathbf{R}}$ where $\bar{\mathbf{R}}$ is diagonal and \mathbf{X} unitary, we have $\xi = \mathbf{X}(\arctan \bar{\mathbf{R}})\mathbf{X}^\dagger$. Using trial functions with asymptotic form

$$\mathbf{F}^t \sim k^{-\frac{1}{2}} \{(\sin x) \cos \xi^t + (\cos x) \sin \xi^t\} \quad (2.24)$$

we put $\delta\xi = -L^t$. The corrected \mathbf{R} matrix is

$$\mathbf{R}^K = [\sin \xi^t + (\cos \xi^t) \delta\xi] [\cos \xi^t - (\sin \xi^t) \delta\xi]^{-1} \quad (2.25)$$

(Seaton 1967).

2.3. Atomic wavefunctions

We first consider a formulation in which closed shells are neglected (closed shells are discussed in §2.6). Configurations np^q contain terms $S_i L_i$ listed in table 1. The wave functions are constructed by using fractional parentage expansions:

$$\Psi(np^q S_i L_i | 1, 2, \dots, q) = \sum_j A_q(i, j) \psi(np^{q-1} S_j L_j np S_i L_i | 1, 2, \dots, q-1; q), \quad (2.26)$$

where the functions on the right-hand side are constructed using vector-coupling formulae as in (2.3). A consistent set of fractional parentage coefficients $A_q(i, j)$ is given in table 2. It should be noted that, in the tables of algebraic coefficients, we use the abbreviated notation

$$A \sqrt{BC} / D \sqrt{EF} = A \sqrt{(BC)} / D \sqrt{(EF)}.$$

The approximate ion functions (2.26) are not eigenfunctions of the ion Hamiltonian $H_q(1, 2, \dots, q)$, but are such that

$$(\Psi(np^q S_i L_i) | H_q | \Psi(np^q S_i L_i)) = \delta(i', i) E(np^q S_i L_i), \quad (2.27)$$

where $E(np^q S_i L_i)$ will be referred to as the calculated ion energy. The energy integrals are evaluated on expanding the electrostatic interactions,

$$\frac{1}{r_{12}} = \sum_\lambda P_\lambda(\hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2) \gamma_\lambda(r_1, r_2), \quad (2.28)$$

where

$$\gamma_\lambda(r_1, r_2) = \begin{cases} r_1^\lambda / r_2^{\lambda+1} & (r_1 < r_2), \\ r_2^\lambda / r_1^{\lambda+1} & (r_2 < r_1). \end{cases} \quad (2.29)$$

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE 83

TABLE 1. TERMS IN np^q CONFIGURATIONS

q	i	$S_i L_i$	q	i	$S_i L_i$
1 and 5	1	2P	3	1	4S
2 and 4	1	3P	6	2	2D
	2	1D		3	2P
	3	1S		1	1S

TABLE 2. FRACTIONAL PARENTAGE COEFFICIENTS

q	i	j	$A_q(i, j)$	q	i	j	$A_q(i, j)$	
1	1	1	1	4	1	1	$1/\sqrt{3}$	
2	1	1	1	5	1	1	$-\sqrt{5}/2\sqrt{3}$	
	2	1	1		2	2	$1/2$	
	3	1	1		2	2	$\sqrt{3}/2$	
3	1	1	1	6	1	1	$1/2$	
		2	1			2	2	-1
		3	1			2	2	$\sqrt{3}/\sqrt{5}$
	2	1	$1/\sqrt{2}$	3	3	1	$1/\sqrt{3}$	
		2	$-1/\sqrt{2}$			2	$+1/\sqrt{15}$	
		3	$-1/\sqrt{2}$			3	1	
3	2	1	$-1/\sqrt{2}$	3	3	1	1	
		2	$-\sqrt{5}/3\sqrt{2}$			2	$1/\sqrt{3}$	
		3	$\sqrt{2}/3$			3	$+1/\sqrt{15}$	

Note. In this table $A_{\sqrt{BC}/D\sqrt{EF}}$ stands for $A_{\sqrt{(BC)}/D\sqrt{(EF)}}$.

TABLE 3. COEFFICIENTS $f_2(p^q, S_i L_i)$

q	i	$f_2(p^q, S_i L_i)$	q	i	$f_2(p^q, S_i L_i)$	
2	1	-0.20	4	1	-0.60	
	2	+0.04		2	-0.36	
	3	+0.40		3	0.00	
3	1	-0.60	5	1	-0.80	
	2	-0.24		6	1	-1.20
	3	0.00				

TABLE 4. COUPLED STATES IN $np^q l S L$

$q = 1$ and 5			$q = 3$			
S	i	l	S	i	l	
0 and 1	1	$L-1$	0	2	$L-1$	
	1	$L+1$		2	$L+1$	
0 and 1	1	L		3	$L-1$	
				3	$L+1$	
$q = 2$ and 4				0	2	$L-2$
S	i	l			2	L
$\frac{1}{2}$	1	$L-1$	2		$L+2$	
	1	$L+1$	3		L	
	2	$L-1$	1		2	$L-1$
	2	$L+1$			2	$L+1$
$\frac{1}{2}$	1	L		3	$L-1$	
	2	$L-2$		3	$L+1$	
	2	L		1	1	L
	2	L			2	$L-2$
$\frac{3}{2}$	2	$L+2$	2		L	
	3	L	2		$L+2$	
$\frac{3}{2}$	1	$L-1$	2		3	L
	1	$L+1$			1	L
$\frac{3}{2}$	1	L				

TABLE 5. THE COEFFICIENTS f_2

i	$l-L$	i'	$l'-L$	$5f_2$ for $q = 1, -5f_2$ for $q = 5$	i	$l-L$	i'	$l'-L$	$5f_2$ for $q = 3$
1	-1	1	-1	$(L-1)/(2L+1)$	2	-1	2	-1	0
1	-1	1	+1	$-3\sqrt{L(L+1)}/(2L+1)$	2	-1	2	+1	0
1	+1	1	+1	$(L+2)/(2L+1)$	2	-1	3	-1	$-3\sqrt{(L^2-1)}/(2L+1)$
1	0	1	0	-1	2	-1	3	+1	$-3\sqrt{(L-1)}/L/(2L+1)$
				$5f_2$ for $q = 2, -5f_2$ for $q = 4$	2	+1	2	+1	0
1	0	1	0	1	2	+1	3	-1	$3\sqrt{(L+1)}/(L+2)/(2L+1)$
2	-2	2	-2	$2(L-2)/(2L-1)$	2	+1	3	+1	$3\sqrt{L(L+2)}/(2L+1)$
2	-2	2	0	$-\sqrt{6(L^2-1)}/(2L+3)/(2L-1)\sqrt{(2L+1)}$	3	-1	3	-1	0
2	-2	3	0	$-2\sqrt{3(L-1)}/L\sqrt{(2L-1)}/(2L+1)$	3	-1	3	+1	0
2	0	2	0	$-(2L-3)/(2L+5)/(2L-1)/(2L+3)$	1	0	1	0	0
2	0	2	2	$-\sqrt{6L(L+2)}/(2L-1)/(2L+3)\sqrt{(2L+1)}$	2	-2	2	-2	0
2	0	3	0	$2\sqrt{2L(L+1)}/\sqrt{(2L-1)}/(2L+3)$	2	-2	2	0	0
2	+2	2	+2	$2(L+3)/(2L+3)$	2	-2	3	0	$-3\sqrt{2(L^2-1)}/\sqrt{(2L-1)}/(2L+1)$
2	+2	3	0	$-2\sqrt{3(L+1)}/(L+2)/\sqrt{(2L+1)}/(2L+3)$	2	0	2	0	0
3	0	3	0	0	2	0	2	+2	0
1	-1	1	-1	$-(L-1)/(2L+1)$	2	0	3	0	$3\sqrt{3}/\sqrt{(2L-1)}/(2L+3)$
1	-1	1	+1	$3\sqrt{L(L+1)}/(2L+1)$	2	+2	2	+2	0
1	+1	1	+1	$-(L+2)/(2L+1)$	2	+2	3	0	$3\sqrt{2L(L+2)}/\sqrt{(2L+1)}/(2L+3)$
2	-1	2	-1	$-(L+5)/(2L+1)$	3	0	3	0	0
2	-1	2	+1	$-3\sqrt{(L-1)}/(L+2)/(2L+1)$					
2	+1	2	+1	$-(L-4)/(2L+1)$					

Note. In this table $A\sqrt{BC}/D\sqrt{EF}$ stands for $A\sqrt{(BC)}/D\sqrt{(EF)}$.

TABLE 6. THE COEFFICIENTS g_λ FOR $q = 1$ AND 5

S	$l-L$	$l'-L$	$\lambda-L$	$(2\lambda+1)g_\lambda$	
				$q = 1$	$q = 5$
0	-1	-1	-2	$-3(L-1)/(2L-1)$	$3(L-1)/(2L-1)$
			0	$-3/(2L-1)/(2L+1)$	$-3L(2L-3)/(2L-1)/(2L+1)$
			0	$3\sqrt{L(L+1)}/(2L+1)$	$6\sqrt{L(L+1)}/(2L+1)$
	+1	+1	0	$-3/(2L+1)/(2L+3)$	$-3(L+1)/(2L+5)/(2L+3)/(2L+1)$
			2	$-3(L+2)/(2L+3)$	$3(L+2)/(2L+3)$
			-1	$3/(2L+1)$	$3L/(2L+1)$
1	-1	-1	-2	$3(L-1)/(2L-1)$	$3(L-1)/(2L-1)$
			0	$3/(2L-1)/(2L+1)$	$3L/(2L-1)$
			0	$-3\sqrt{L(L+1)}/(2L+1)$	0
	+1	+1	0	$3/(2L+1)/(2L+3)$	$3(L+1)/(2L+3)$
			2	$3(L+2)/(2L+3)$	$3(L+2)/(2L+3)$
			-1	$-3/(2L+1)$	$3L/(2L+1)$
0	0	+1	$3/(2L+1)$	$3(L+1)/(2L+1)$	

Note. In this table $A\sqrt{BC}/D\sqrt{EF}$ stands for $A\sqrt{(BC)}/D\sqrt{(EF)}$.

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE 85

TABLE 7. THE COEFFICIENTS g_λ FOR $q = 2$ AND 4

S	i	$l-L$	i'	$l'-L$	$\lambda-L$	$(2\lambda+1) g_\lambda$	
						$q = 2$	$q = 4$
$\frac{1}{2}$	1	0	1	0	-1	$-3L/2(2L+1)$	$-3(L+3)/2(2L+1)$
					+1	$-3(L+1)/2(2L+1)$	$3(2-L)/2(2L+1)$
	1	0	2	-2	-1	$3\sqrt{3(L^2-1)}/\sqrt{2(2L-1)}(2L+1)$	$3\sqrt{3(L^2-1)}/\sqrt{2(2L-1)}(2L+1)$
					-1	$3(L-2)\sqrt{(2L+3)}/2(2L+1)\sqrt{(2L-1)}$	$-3(L+1)\sqrt{(2L+3)}/2(2L+1)\sqrt{(2L-1)}$
	1	0	2	0	-1	$-3(L+3)\sqrt{(2L-1)}/2(2L+1)\sqrt{(2L+3)}$	$3L\sqrt{(2L-1)}/2(2L+1)\sqrt{(2L+3)}$
					+1	$-3\sqrt{3L(L+2)}/\sqrt{2(2L+1)}(2L+3)$	$-3\sqrt{3L(L+2)}/\sqrt{2(2L+1)}(2L+3)$
	1	0	3	0	-1	$3\sqrt{L(L+1)}/(2L+1)\sqrt{2}$	$-3\sqrt{L(L+1)}/(2L+1)\sqrt{2}$
					+1	$-3\sqrt{L(L+1)}/(2L+1)\sqrt{2}$	$3\sqrt{L(L+1)}/(2L+1)\sqrt{2}$
	2	-2	2	-2	-3	$3(L-2)/(2L-3)$	$3(L-2)/(2L-3)$
					-1	$3/(2L-3)(2L-1)$	$6(L-1)/(2L-3)(2L-1)$
	2	-2	2	0	-1	$-\sqrt{3(L^2-1)}(2L+3)/(2L-1)\sqrt{2(2L+1)}$	$\sqrt{3(L^2-1)}(2L+3)/(2L-1)\sqrt{2(2L+1)}$
					-1	$-\sqrt{3(L-1)}L/\sqrt{(2L-1)}(2L+1)$	$\sqrt{3(L-1)}L/\sqrt{(2L-1)}(2L+1)$
	2	-2	3	0	-1	$(12-13L+2L^2)/2(2L-1)(2L+1)$	$(10L^2-11L-3)/2(2L-1)(2L+1)$
					+1	$(27+17L+2L^2)/2(2L+1)(2L+3)$	$(10L^2+31L+18)/2(2L+1)(2L+3)$
	2	0	2	+2	+1	$-\sqrt{3L(L+2)}(2L-1)/(2L+3)\sqrt{2(2L+1)}$	$\sqrt{3L(L+2)}(2L-1)/(2L+3)\sqrt{2(2L+1)}$
					-1	$\sqrt{L(L+1)}(2L+3)/(2L+1)\sqrt{2(2L-1)}$	$-\sqrt{L(L+1)}(2L+3)/(2L+1)\sqrt{2(2L-1)}$
	2	0	3	0	+1	$\sqrt{L(L+1)}(2L-1)/(2L+1)\sqrt{2(2L+3)}$	$-\sqrt{L(L+1)}(2L-1)/(2L+1)\sqrt{2(2L+3)}$
					+1	$3/(2L+5)(2L+3)$	$-6(L+2)/(2L+3)(2L+5)$
2	+2	2	+2	+1	$3(L+3)/(2L+5)$	$3(L+3)/(2L+5)$	
				+1	$-\sqrt{3(L+1)}(L+2)/\sqrt{(2L+1)}(2L+3)$	$\sqrt{3(L+1)}(L+2)/\sqrt{(2L+1)}(2L+3)$	
3	0	3	0	-1	$L/(2L+1)$	$2L/(2L+1)$	
				+1	$(L+1)/(2L+1)$	$2(L+1)/(2L+1)$	
$\frac{1}{2}$	1	-1	1	-1	-2	$-3(L-1)/2(2L-1)$	$3(L-1)/(2L-1)$
					0	$-3L/(2L-1)(2L+1)$	$-3(L-1)(2L+3)/2(2L-1)(2L+1)$
	1	-1	1	+1	0	$-3\sqrt{L(L+1)}/2(2L+1)$	$-9\sqrt{L(L+1)}/2(2L+1)$
					-2	$3\sqrt{3(L^2-1)}/2(2L-1)$	0
	1	-1	2	-1	0	$-3\sqrt{3(L^2-1)}/(2L-1)(2L+1)$	$3\sqrt{3(L^2-1)}/2(2L+1)$
					0	$-3\sqrt{3(L+1)}(L+2)/2(2L+1)$	$-3\sqrt{3(L+1)}(L+2)/2(2L+1)$
	1	+1	1	+1	0	$3(L+1)/(2L+1)(2L+3)$	$-3(L+2)(2L-1)/2(2L+1)(2L+3)$
					+2	$-3(L+2)/2(2L+3)$	$3(L+2)/(2L+3)$
	1	+1	2	-1	0	$3\sqrt{3(L-1)}L/2(2L+1)$	$3\sqrt{3(L-1)}L/2(2L+1)$
					0	$-3\sqrt{3L(L+2)}/(2L+1)(2L+3)$	$-3\sqrt{3L(L+2)}/2(2L+1)$
	1	+1	2	+1	+2	$-3\sqrt{3L(L+2)}/2(2L+3)$	0
					-2	$3(L-3)/2(2L-1)$	$3(L-1)/(2L-1)$
	2	-1	2	-1	-2	$3(L-3)/2(2L-1)$	$3(L-1)/(2L-1)$
					0	$3(L+2)/(2L-1)(2L+1)$	$3(2L^2+5L-1)/2(2L-1)(2L+1)$
	2	-1	2	+1	0	$-3\sqrt{(L-1)}(L+2)/2(2L+1)$	$3\sqrt{(L-1)}(L+2)/2(2L+1)$
					0	$-3(L-1)/(2L+1)(2L+3)$	$3(2L^2-L-4)/2(2L+1)(2L+3)$
	2	+1	2	+1	+2	$3(L+4)/2(2L+3)$	$3(L+2)/(2L+3)$
					-2	$3(L+4)/2(2L+3)$	$3(L+2)/(2L+3)$
$\frac{3}{2}$	1	0	1	0	-1	$3L/(2L+1)$	$3L/(2L+1)$
					+1	$3(L+1)/(2L+1)$	$3(L+1)/(2L+1)$
$\frac{3}{2}$	1	-1	1	-1	-2	$3(L-1)/(2L-1)$	$3(L-1)/(2L-1)$
					0	$6L/(2L-1)(2L+1)$	$3L/(2L-1)$
	1	-1	1	+1	0	$3\sqrt{L(L+1)}/(2L+1)$	0
					0	$-6(L+1)/(2L+1)(2L+3)$	$3(L+1)/(2L+3)$
1	+1	1	+1	+2	$3(L+2)/(2L+3)$	$3(L+2)/(2L+3)$	

Note. In this table $A\sqrt{BC}/D\sqrt{EF}$ stands for $A\sqrt{(BC)}/D\sqrt{(EF)}$.

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE 87

We introduce
$$y_\lambda(AC|r_2) = \int_0^\infty A(r_1) C(r_1) \gamma_\lambda(r_1, r_2) dr_1 \quad (2.30)$$

and
$$R_\lambda(ABCD) = \int_0^\infty y_\lambda(AC|r_2) B(r_2) D(r_2) dr_2 \\ = \int_0^\infty A(r_1) C(r_1) y_\lambda(BD|r_1) dr_1, \quad (2.31)$$

where A , B , C and D are radial functions. Denoting the np radial function in $np^q S_i L_i$ by P_i we obtain

$$E(np^q S_i L_i) = q \left(P_i \left| -\frac{d^2}{dr^2} + \frac{2}{r^2} - \frac{2Z}{r} \right| P_i \right) + q(q-1) R_0(P_i^4) + 2f_2(p^q, S_i L_i) R_2(P_i^4), \quad (2.32)$$

where the coefficients* $f_2(p^q, S_i L_i)$ are given in table 3. The Hartree-Fock equation for P_i is

$$\left[-\left(\frac{d^2}{dr^2} - \frac{2}{r^2} \right) - \frac{2Z}{r} + 2(q-1) y_0(P_i^2|r) + \frac{4}{q} f_2(p^q, S_i L_i) y_2(P_i^2|r) + \epsilon_i \right] P_i = 0. \quad (2.33)$$

The differences between the radial functions P_i for different terms $S_i L_i$ are not large. We greatly simplify the problem by neglecting these differences. Our procedure is to use a radial function P obtained on solving the equation

$$[\mathcal{L}_1 - 2y_0(P^2|r) + \epsilon] P = 0, \quad (2.34)$$

where
$$\mathcal{L}_1 = -\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) - \frac{2Z}{r} + 2qy_0(P^2|r) \quad (2.35)$$

and where terms in y_2 are neglected. Substituting this function in (2.32) we obtain

$$E(np^q S_i L_i) = \bar{E}(np^q) + 2f_2(p^q, S_i L_i) R_2(P^4), \quad (2.36)$$

where
$$\bar{E}(np^q) = -q(q-1) R_0(P^4) - q\epsilon. \quad (2.37)$$

The total energy in the collision problem is

$$E = E(np^q S_i L_i) + k_i^2. \quad (2.38)$$

Putting
$$E = \bar{E}(np^q) + k^2, \quad (2.39)$$

which defines k^2 , we have

$$k_i^2 = k^2 - 2f_2(p^q, S_i L_i) R_2(P^4). \quad (2.40)$$

2.4. Wave functions for the collision problem

The main approximation made in our work is to retain in (2.5) only those ion states which belong to the np^q configuration. The significance of this approximation will be discussed further in a later paper in the present series.

In table 4 we list the states in $np^q S_i L_i lSL$. For each value of SL we have two groups of coupled states, of different parity. The algebraic reductions are greatly simplified if the orbitals for the colliding electron are taken to be orthogonal to the orbitals for the ionic electrons. Suppose that we have a function (2.2) with $l = 1$ and that we construct the anti-symmetric function

$$\Phi(np^q S_i L_i pSL) \quad (2.41)$$

* The coefficients for $q = 2$ are given incorrectly in the paper by Saraph *et al.* (1966).

by using (2.3) and (2.4). If we now take the radial function F in (2.2) to be equal to P , (2.41) must be proportional to $\Psi(np^{q+1}SL)$, where it is to be understood that $\Psi(np^{q+1}SL)$ vanishes if SL is not allowed in np^{q+1} . Since an arbitrary radial function F may be written as a linear combination of P and of a function orthogonal to P , we may take the complete wave function to be of the form

$$\Psi_{i'l'} = \sum_{il} \Phi_{i'l'}(np^q S_i L_i l SL) + \alpha' \Psi(np^{q+1}SL), \quad (2.42)$$

where it is to be understood that radial functions $F_{il, i'l'}$ for $l = 1$ are orthogonal to P , and that the last term is to be omitted if functions with $l = 1$ do not occur.

2.5. Reduction of integrals

Using (2.42) we have

$$\begin{aligned} L_{i'l', i'l'} = & \sum_{ii'l'} (\Phi'(i'l') | H - E | \Phi(il)) + \alpha \sum_{i'l'} (\Phi'(i'l') | H - E | \Psi(np^{q+1}SL)) \\ & + \alpha' \sum_{il} (\Psi(np^{q+1}SL) | H - E | \Phi(il)) + \alpha' \alpha (\Psi(np^{q+1}SL) | H - E | \Psi(np^{q+1}SL)), \end{aligned} \quad (2.43)$$

where we write $\Phi'(i'l')$ for $\Phi_{i'l'}(i'l')$ and $\Phi(il)$ for $\Phi_{i'l'}(il)$. Using (2.4) we obtain

$$\begin{aligned} (\Phi'(i'l') | H - E | \Phi(il)) = & (\varphi(i'l' | (q+1)^{-1}; q+1) | H - E | \varphi(il | (q+1)^{-1}; q+1)) \\ & - q(\varphi(i'l' | (q+1)^{-1}; q+1) | H - E | \varphi(il | q^{-1}; q)) \end{aligned} \quad (2.44)$$

where the first term on the right-hand side is a direct integral and the second is an exchange integral. Using (2.27) we readily see that the operator $(H - E)$ in the direct integral may be replaced by

$$H_1(q+1) - k_i^2 + \sum_{t=1}^q \frac{1}{r_{t, q+1}},$$

where $H_1(q+1) = -(\nabla_{q+1}^2 + 2Z/r_{q+1})$. When we use orbitals for the colliding electron which are orthogonal to the orbitals for the ionic electrons, the only term in $(H - E)$ which gives a non-zero contribution to the exchange integral is $1/r_{q, q+1}$.

For $q = 1$ Percival & Seaton (1957) obtain

$$\begin{aligned} (\Phi'(i'l') | H - E | \Phi(il)) = & (F'_{i'l'} | \mathcal{L}_l - k_i^2 | F_{il}) \delta(i'l', il) \\ & + 2f_2(pl' pl; L) R_2(PF'_{i'l'} PF_{il}) - (-1)^{1-s} 2 \sum_{\lambda} g_{\lambda}(pl' pl; L) R_{\lambda}(PF'_{i'l'} F_{il} P) \end{aligned} \quad (2.45)$$

and tabulate expressions for the coefficients $f_2(pl' pl; L)$ and $g_{\lambda}(pl' pl; L)$. For $q > 1$ we use fractional parentage expansions and introduce transformations which interchange coupling orders, so as to obtain states in which the angular momenta are coupled for the electrons with coordinates q and $q+1$. We obtain

$$\begin{aligned} (\Phi'(i'l') | H - E | \Phi(il)) = & (F'_{i'l'} | \mathcal{L}_l - k_i^2 | F_{il}) \delta(i'l', il) \\ & + 2f_2(i'l', il; L) R_2(PF'_{i'l'} PF_{il}) - 2 \sum_{\lambda} g_{\lambda}(i'l', il; SL) R_{\lambda}(PF'_{i'l'} F_{il} P), \end{aligned} \quad (2.46)$$

where

$$f_2(i'l', il; L) = \delta(S_{i'}, S_i) q[(2L_{i'} + 1)(2L_i + 1)]^{\frac{1}{2}} \\ \times \sum_j A_q(i', j) A_q(i, j) \sum_{\mathcal{L}} (2\mathcal{L} + 1) W(L_j 1Ll'; L_{i'} \mathcal{L}) W(L_j 1Ll; L_i \mathcal{L}) f_2(pl'pl; \mathcal{L}) \quad (2.47)$$

$$\text{and } g_\lambda(i'l', il; SL) = q[(2L_{i'} + 1)(2L_i + 1)(2S_{i'} + 1)(2S_i + 1)]^{\frac{1}{2}} \\ \times \sum_j A_q(i', j) A_q(i, j) W(S_{i'} \frac{1}{2} \frac{1}{2} S_{i'}; SS_j) \\ \times \sum_{\mathcal{L}} (2\mathcal{L} + 1) W(L_j 1Ll'; L_{i'} \mathcal{L}) W(L_j 1Ll; L_i \mathcal{L}) g_\lambda(pl'pl; \mathcal{L}) \quad (2.48)$$

and where W is a Racah coefficient. Reduced expressions for the coefficients f_2 and g_λ , for each transition, as a function of L , are given in tables 5, 6, 7 and 8.

The remaining integrals in (2.43) are evaluated without difficulty. Using (2.4) we obtain

$$(\Phi'(i'l') | H - E | \Psi(np^{q+1}SL)) = (q+1)^{\frac{1}{2}} (\varphi'(i'l') | (q+1)^{-1}; q+1 | H - E | \Psi(np^{q+1}SL)) \quad (2.49)$$

and on making a fractional parentage expansion of $\Psi(np^{q+1}SL)$ we obtain integrals similar to the direct integral in (2.44). Using (2.34) we obtain the final result

$$(\Phi'(i'l') | H - E | \Psi(np^{q+1}SL)) = (q+1)^{\frac{1}{2}} [2d_0(i'l', SL) R_0(P^3 F'_{i'l'}) + 2d_2(i'l', SL) R_2(P^3 F'_{i'l'})] \quad (2.50)$$

$$\text{where } d_0(i'l', SL) = \delta(l', 1) A_{q+1}(SL, i'), \quad (2.51)$$

$$d_2(i'l', SL) = \sum_i A_{q+1}(SL, i) f_2(i'l', il; L). \quad (2.52)$$

$$\text{The integral } (\Psi(np^{q+1}SL) | H | \Psi(np^{q+1}SL)) \quad (2.53)$$

is the expectation value for the energy of np^{q+1} calculated using the radial function for np^q . Using (2.32), (2.34) and (2.39) we obtain

$$(\Psi(np^{q+1}SL) | H - E | \Psi(np^{q+1}SL)) = -(\epsilon + k^2) + 2R_0(P^4) + 2f_2(p^{q+1}, SL) R_2(P^4). \quad (2.54)$$

The parameters α' , α in (2.43) are determined from the variational principle,

$$\frac{\partial}{\partial \alpha'} L_{i'l', i'l'} = \frac{\partial}{\partial \alpha} L_{i'l', i'l'} = 0. \quad (2.55)$$

The final expression for L is then

$$L_{i'l', i'l'} = \sum_{il} (F'_{il} | \mathcal{L}_l - k_i^2 | F_{il}) \\ + 2 \sum_{i'l' il} \{ f_2(i'l', il; L) R_2(PF'_{i'l'} PF_{il}) - \sum_{\lambda} g_\lambda(i'l', il; SL) R_\lambda(PF'_{i'l'} F_{il} P) \} \\ + \frac{4(q+1) \{ \sum_{i'l'} \sum_{\lambda} d_\lambda(i'l', SL) R_\lambda(P^3 F'_{i'l'}) \} \{ \sum_{il} \sum_{\lambda} d_\lambda(il, SL) R_\lambda(P^3 F_{il}) \}}{(\epsilon + k^2) - 2R_0(P^4) - 2f_2(p^{q+1}, SL) R_2(P^4)}. \quad (2.56)$$

The algebraic calculations in the work of Seaton (1953*a, b*) were made on expressing all functions as linear combinations of Slater determinants and using methods described by Condon & Shortley (1935). Such calculations are very tedious for hand calculations but, as pointed out by Godfredsen (1966), they can be programmed in a systematic way for a computer. The method of the present paper, using fractional parentage coefficients, becomes

extremely complicated if one wishes to include configurations containing two or more incomplete shells. In such cases computer calculations using a representation of Slater determinants are to be preferred. Dr W. Eissner and Dr H. Nussbaumer, of University College London, have developed very general computer programs for the algebraic formulation of collision problems using this method, and these programs have been used for checking all of the coefficients given in the present paper.

Expressions for the coefficients for $l' = l$ have previously been obtained by Yamanouchi & Amemiya (1946) and these are quoted in full by Slater (1960). We find that, for each value of q and l , constants must be added to their diagonal elements in order to obtain agreement with our results. When this is done, our results agree in all cases with those of Yamanouchi and Amemiya, but it is found that there is one misprint in Slater's tables ($g_L(1, L-1, 2, L-1; \frac{1}{2}, L)$ for $q = 4$).

2.6. Radial equations

On imposing the condition that $[\rho - \mathbf{L}]$ should be stationary for all variations of the radial functions, we obtain the radial equations

$$\begin{aligned} (\mathcal{L}_l - k_l^2) F_{i'l'} + 2 \sum_{il} f_2(i'l', il; L) y_2(P^2) F_{il} + \left\{ -2 \sum_{il} \sum_{\lambda} g_{\lambda}(i'l', il; SL) y_{\lambda}(PF_{il}) + \delta(l', 1) \mu(i') \right. \\ \left. + \frac{4(q+1) \left[\sum_{il} \sum_{\lambda} d_{\lambda}(il, SL) R_{\lambda}(P^3 F_{il}) \right] \sum_{\lambda} d_{\lambda}(i'l', SL) y_{\lambda}(P^2)}{(\epsilon + k^2) - 2R_0(P^4) - 2f_2(p^{q+1}, SL) R_2(P^4)} \right\} P = 0, \quad (2.57) \end{aligned}$$

where the parameter $\mu(i')$ is adjusted so as to make $F_{i'l'}$ orthogonal to P for $l' = 1$.

Closed shells are taken into account by redefining the operator \mathcal{L}_l . If, in place of np^q , we consider $1s^2 2s^2 2p^q$ for $n = 2$ and $1s^2 2s^2 2p^6 3s^2 3p^q$ for $n = 3$, the definition (2.35) of \mathcal{L}_l is replaced by

$$\mathcal{L}_l = \mathcal{L}_l^{(0)} - W, \quad (2.58)$$

where

$$\mathcal{L}_l^{(0)} = - \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) - \frac{2Z}{r} + \sum_{m=1}^2 4y_0(S_m^2) + 2qy_0(P^2) + \delta(n, 3) [12y_0(P_2^2) + 4y_0(S_3^2)] \quad (2.59)$$

and

$$\begin{aligned} WF_l = \frac{2}{(2l+1)} \left\{ \sum_{m=1}^2 y_l(S_m F_l) S_m + \delta(n, 3) y_l(S_3 F_l) S_3 \right. \\ \left. + \delta(n, 3) \left[\frac{3l}{(2l-1)} y_{l-1}(P_2 F_l) + \frac{(3l+3)}{(2l+3)} y_{l+1}(P_2 F_l) \right] P_2 \right\} \quad (2.60) \end{aligned}$$

(Salmona & Seaton 1961). In these expressions, S_m is the ms radial function and, for $n = 3$, P_2 is the $2p$ radial function. When closed shells are included additional Lagrange multipliers must be included in (2.57).

The coupled equations (2.57) could be solved exactly but we doubt whether the effort would be justified. Our procedure is to obtain wave functions in approximations which involve the omission of certain smaller terms in the equations (2.57), and then to correct the calculated ρ matrices using variational expressions in which no terms are neglected. This procedure reduces considerably the length and complexity of the calculations. We believe that the results obtained should approximate closely to those which would be obtained

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE 91

from exact solutions of the coupled equations, and that any error introduced will be small compared with the errors which result from our main approximation, neglect of coupling to configurations other than $2p^q$.

2.7. *The exact resonance approximation*

In previous work (Seaton 1953*a, b*) it has been found that, for $2p^q$ configurations, the dominant contributions to the collision strengths come from the p -waves, $l' = l = 1$. For the p -waves (2.57) contains terms in $\lambda = 0, 1$ and 2 and it is found that the $\lambda = 0$ exchange coupling terms may be large. In the exact resonance approximation we calculate wave functions in the approximation of neglecting all $\lambda = 2$ terms in the calculation of ion energies, and in the equations (2.57). In this approximation all terms $S_i L_i$ in np^q have equal energies, and it is found that the equations for the radial functions can be uncoupled. From the solutions of these equations we construct trial functions with allowance for energy differences, and use these to calculate the corrected matrices ρ^K with inclusion of $\lambda = 2$ terms. It should be noted that this procedure is fully consistent with the procedure described in §(2.3) for the calculation of ion functions and ion energies.

Consistently neglecting $\lambda = 2$ terms we have $k_i^2 = k^2$ and, for $l' = l = 1$, equation (2.57) reduces to

$$(\mathcal{L}_1 - k^2) F_{i'} + \left\{ -2 \sum_i g_0(i', i) y_0(PF_i) + \mu(i') + \frac{4(q+1) d_0(i') y_0(P^2) \sum_i d_0(i) R_0(P^3 F_i)}{(\epsilon + k^2) - 2R_0(P^4)} \right\} P = 0. \quad (2.61)$$

$$\text{It may be shown that} \quad g_0(i', i) = \delta(i', i) - (q+1) d_0(i') d_0(i) \quad (2.62)$$

and hence that (2.61) may be written

$$(\mathcal{L}_1 - k^2) F_{i'} + \mu(i') P - 2y_0(PF_{i'}) P + 2(q+1) d_0(i') \sum_i d_0(i) \left\{ y_0(PF_i) + \frac{2R_0(P^3 F_i) y_0(P^2)}{(\epsilon + k^2) - 2R_0(P^4)} \right\} P = 0. \quad (2.63)$$

An explicit expression for $\mu(i')$ is obtained on multiplying (2.63) by P and integrating. Using (2.34) we obtain

$$\mu(i') = -2(q+1) d_0(i') \sum_i d_0(i) R_0(P^3 F_i) \left\{ 1 + \frac{2R_0(P^4)}{(\epsilon + k^2) - 2R_0(P^4)} \right\} \quad (2.64)$$

and hence

$$(\mathcal{L}_1 - k^2) F_{i'} - 2y_0(PF_{i'}) P + 2(q+1) d_0(i') \sum_i d_0(i) \left\{ y_0(PF_i) - R_0(P^3 F_i) + \frac{2R_0(P^3 F_i) [y_0(P^2) - R_0(P^4)]}{(\epsilon + k^2) - 2R_0(P^4)} \right\} P = 0. \quad (2.65)$$

If SL is not allowed in p^{q+1} we have $d_0(i) = 0$ for all i . In this case the equations (2.65) reduce to a single uncoupled equation. Putting $F_i = \mathcal{F}$ we have

$$(\mathcal{L}_1 - k^2) \mathcal{F} - 2y_0(P\mathcal{F}) P = 0. \quad (2.66)$$

If SL is allowed in p^{q+1} the solutions of the coupled equations (2.65) may be expressed in terms of two functions, \mathcal{F} and \mathcal{G} . Introducing functions $b(i)$ such that

$$\sum_i b(i) d_0(i) = 0, \quad \sum_i b^2(i) = 1 \quad (2.67)$$

it is readily shown that the functions $F_i = b(i)\mathcal{F}$ (2.68)

are solutions of (2.65). A second set of solutions is given by

$$F_i = d_0(i) g. \quad (2.69)$$

Substituting (2.69) in (2.65), and using the fact that $\sum_i d_0^2(i) = 1$, which follows from (2.51), we obtain

$$(\mathcal{L}_1 - k^2) g + 2qy_0(Pg) P + \frac{2(q+1) R_0(P^3g) [2y_0(P^2) - (\epsilon + k^2)] P}{(\epsilon + k^2) - 2R_0(P^4)} = 0. \quad (2.70)$$

The function \mathcal{G} is defined by $\mathcal{G} = g + \frac{2R_0(P^3\mathcal{G}) P}{(\epsilon + k^2)}$. (2.71)

Since P is orthogonal to g , we obtain

$$(P|\mathcal{G}) = \frac{2R_0(P^3\mathcal{G})}{(\epsilon + k^2)}, \quad (2.72)$$

and substituting (2.71) in (2.70) we obtain

$$(\mathcal{L}_1 - k^2) \mathcal{G} + 2q[y_0(P\mathcal{G}) - R_0(P^3\mathcal{G})] P = 0. \quad (2.73)$$

The equations for \mathcal{F} and \mathcal{G} may be combined into a single equation

$$(\mathcal{L}_1 - k^2) \phi + 2ty_0(P\phi) P + \eta P = 0, \quad (2.74)$$

where η is such that $(1+q)(\epsilon+k^2)(P|\phi) = 2(1+t)R_0(P^3\phi)$. (2.75)

The function ϕ is then equal to \mathcal{F} for $t = -1$ and to \mathcal{G} for $t = q$.

In order to calculate ρ^K , without neglect of $\lambda = 2$ terms, we must construct trial functions with asymptotic form

$$F_{i'i}^l \sim k_i^{-\frac{1}{2}} \{ \sin(x_{i'} + \tau_{i'}) \delta(i', i) + \cos(x_{i'} + \tau_{i'}) \rho_{i'i}^l \}. \quad (2.76)$$

To do this, we solve the equations for \mathcal{F} and \mathcal{G} for each of the energies k_i^2 . The solutions are denoted by \mathcal{F}_i and \mathcal{G}_i and are taken to have asymptotic form

$$\left. \begin{aligned} \mathcal{F}_i &\sim k_i^{-\frac{1}{2}} \{ \sin(x_i + \tau_i) + \cos(x_i + \tau_i) \rho_i(\mathcal{F}_i) \}, \\ \mathcal{G}_i &\sim k_i^{-\frac{1}{2}} \{ \sin(x_i + \tau_i) + \cos(x_i + \tau_i) \rho_i(\mathcal{G}_i) \}. \end{aligned} \right\} \quad (2.77)$$

Putting $G_i = g_i - \mathcal{F}_i = \mathcal{G}_i - (P|\mathcal{G}_i) P - \mathcal{F}_i$ (2.78)

we can readily verify that $F_{i'i}^l = \mathcal{F}_{i'} \delta(i', i) + G_{i'} d_0(i') d_0(i)$ (2.79)

is a solution of (2.63), with $k^2 = k_i^2$, and has asymptotic form (2.76), and that

$$\rho_{i'i}^l = \rho_{i'}(\mathcal{F}_{i'}) \delta(i', i) - [\rho_{i'}(\mathcal{F}_{i'}) - \rho_{i'}(\mathcal{G}_{i'})] d_0(i') d_0(i). \quad (2.80)$$

The final results for ρ^K in the exact resonance approximation are obtained on substituting the functions (2.79) into the full expression (2.56) for the \mathbf{L} matrix. It may be noted that, in this approximation, ρ^K is symmetric but ρ^l is not symmetric. The exact resonance approximation will be referred to as the e.r. approximation.

2.8. *The distorted wave approximation*

In the distorted wave approximation the wave functions are calculated neglecting coupling terms and exchange terms. This is used for all partial waves other than the p -waves. For the more highly ionized systems it can also be used for the p -waves.

In this approximation we solve the equations

$$(\mathcal{L}_i^{(0)} - k_i^2) f_{il} = 0, \quad (2.81)$$

where $\mathcal{L}_i^{(0)}$ is defined by (2.59), and take the solutions to have asymptotic form

$$f_{il} \sim k_i^{-\frac{1}{2}} \sin(x_{il} + \tau_{il}). \quad (2.82)$$

It should be noted that this defines the choice of the phase τ_{il} adopted in all of our work. From the solutions of (2.81) we construct orthogonalized functions

$$F_{il} = f_{il} - \delta(l, 0) \sum_{m=1}^2 (S_m | f_{il}) S_m - \delta(l, 1) (P | f_{il}) P - \delta(n, 3) [\delta(l, 0) (S_3 | f_{il}) S_3 + \delta(l, 1) (P_2 | f_{il}) P_2] \quad (2.83)$$

and trial functions to obtain

$$F_{i'l', il}^t = \delta(i'l', il) F_{il} \quad (2.84)$$

$$\begin{aligned} L_{i'l', il}^t &= \delta(i'l', il) (F_{il} | \mathcal{L}_i - k_i^2 | F_{il}) \\ &+ 2f_2(i'l', il; L) R_2(PF_{i'l'} PF_{il}) - 2 \sum_{\lambda} g_{\lambda}(i'l', il; SL) R_{\lambda}(PF_{i'l'} F_{il} P) \\ &+ \frac{4(q+1) [\sum_{\lambda} d_{\lambda}(i'l', SL) R_{\lambda}(P^3 F_{i'l'})] [\sum_{\lambda} d_{\lambda}(il, SL) R_{\lambda}(P^3 F_{il})]}{(\epsilon + k^2) - 2R_0(P^4) - 2f_2(p^{q+1}, SL) R_2(P^4)}. \end{aligned} \quad (2.85)$$

The distorted wave approximation will be referred to as the d.w. approximation.

2.9. *Energy variation of the collision strengths*

In LS coupling, p^q configurations with $q = 2, 3$ and 4 contain three terms, $S_i L_i$, $i = 1, 2$ and 3 in order of increasing excitation energy. All of our e.r. and d.w. calculations are made for energies such that $k_3^2 \geq 0$, and results for $k_3^2 < 0$ are obtained by extrapolation techniques.

For $k_3^2 \geq 0$ the collision strengths vary slowly as functions of the energy but, for $k_3^2 < 0$, $\Omega(1, 2)$ contains infinite series of resonances, converging on level 3 (Gailitis 1963; Bely *et al.* 1963; Seaton 1966). For astrophysical applications we require reaction rates calculated for Maxwellian distributions of electron energies. If it can be assumed that the Maxwell distribution function does not vary significantly over energy intervals comparable with the widths and separations of the resonances, it is permissible to average over resonance structures before integrating over the Maxwell distribution functions. The collision strengths $\Omega(1, 2)$, averaged over resonance structures in the region $k_3^2 \geq 0$, $k_3^2 < 0$, will be denoted by $\bar{\Omega}(1, 2)$.

We introduce channel indices $\alpha = (S_i L_i l SL)$ and say that α is open if $k_{\alpha}^2 > 0$, and closed if $k_{\alpha}^2 < 0$. Channel $\alpha = (S_i L_i l SL)$ is said to be non-degenerate if only one value of l is allowed for fixed values of $S_i L_i$, SL and parity. Suppose that we have one non-degenerate closed

channel c , and a number of open channels α, β, \dots . It is shown by Gailitis (1963) that

$$\langle |S_{\alpha\beta}|^2 \rangle = |S_{\alpha\beta}^>|^2 + \frac{|S_{\alpha c}^>|^2 |S_{c\beta}^>|^2}{1 - |S_{cc}^>|^2}, \quad (2.86)$$

where $\langle |S_{\alpha\beta}|^2 \rangle$ is equal to $|S_{\alpha\beta}|^2$ averaged over resonances, and where $|S_{mn}^>|^2$ is obtained on calculating $|S_{mn}|^2$ in the region for which all channels are open, and extrapolating to the region in which channel c is closed.

For $q = 2$ and 4 we have $S_3 L_3 = {}^1S$, which gives non-degenerate channels. For $q = 3$ we have $S_3 L_3 = {}^2P$ which can give degenerate channels, but from an examination of the states listed in table 4 it may be seen that, for $q = 3$, $S_3 L_3$ gives non-degenerate channels for all of those states for which there is coupling between $S_1 L_1$ and $S_2 L_2$. It follows that, for $q = 2, 3$ and 4 , the Gailitis formula (2.86) may be used to calculate $\bar{\Omega}(1, 2)$.

Values of $\bar{\Omega}(1, 2)$ are given in the present paper and a further discussion of resonance structures will be given in a later paper.

2.10. Discussion of the formulation

The present formulation is superior, in the following respects, to that used in earlier work:

(i) The use of wave functions of the form (2.42), in which the orbitals for the colliding electrons are orthogonal to the orbitals for the ionic electrons, enables us to evaluate the \mathbf{L} matrix without introducing subsidiary approximations. All 'post-prior' discrepancies are thus avoided.

(ii) Results of approximate calculations are corrected using variational methods, and these methods are such that reciprocity and conservation conditions are satisfied exactly. In the work of Seaton (1953*a, b*, 1955*a*) approximate calculations were corrected using iterative methods, which are less powerful. In some later work (Seaton 1958) variational corrections to the \mathbf{S} matrix were introduced, but that work is unsatisfactory in that the corrected \mathbf{S} matrices are not unitary.

(iii) The variational principle for ρ , with a suitable choice of τ , is much superior to a variational principle for \mathbf{R} . Also, in all approximations, the parameter α in (2.42) is determined variationally. This improves the accuracy of the trial functions.

(iv) In the e.r. approximation, wave functions are calculated with inclusion of exchange interactions with the core and, in calculating variational corrections, full allowance is made for energy differences. In the d.w. approximation, energy differences are allowed for and exchange interactions are included for all partial waves in calculating ρ^k .

(v) Results for $k_3^2 < 0$ are obtained by extrapolation techniques.

3. CALCULATIONS

3.1. Numerical and computational procedures

(a) Ion wave functions and ion energies

Our first calculations for O^{2+} (Shemming 1965) were made using ion functions interpolated from the tables of Hartree, Hartree & Swirls (1939). All subsequent calculations were made by using ion functions calculated by means of a Fortran computer program of Professor Charlotte Froese-Fischer (Froese 1967); we are greatly indebted to her for

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE 95

providing this program and for writing a supplementary program needed to give radial functions in a form convenient for our work. We are also indebted to Dr M. Wilson and Dr S. Budd for their kind and ready co-operation in running this program for us on the I.B.M. 7090 Computer at Imperial College, London.

Table 9 gives values of the integrals $R_2(P^4)$ required for the calculations of energy differences between $2p^q S_i L_i$ terms, and table 10 gives some results for energy differences in O^+ and O^{2+} . The energy differences obtained using our method (§2), in which $\lambda = 2$ terms are neglected in calculating the radial functions, are seen to differ by, at most, 3% from the energy differences obtained by Froese (1967), who retains the $\lambda = 2$ terms in the wave function calculations. The differences between the calculated and experimental energy differences are seen to be much larger than this. Throughout the present paper, calculated energy differences have been used.

TABLE 9. THE INTEGRALS $R_2(P^4)$ FOR $2p^q$ IONS

$q = 1$		$q = 2$		$q = 3$		$q = 4$		$q = 5$	
ion	R_2	ion	R_2	ion	R_2	ion	R_2	ion	R_2
C^+	0.2885	N^+	0.3331	O^+	0.3775	F^+	0.4217	Ne^+	0.4658
N^{2+}	0.3818	O^{2+}	0.4263	F^{2+}	0.4706	Ne^{2+}	0.5149	Na^{2+}	0.5590
O^{3+}	0.4731	F^{3+}	0.5176	Ne^{3+}	0.5621	Na^{3+}	0.6064	Mg^{3+}	0.6507
F^{4+}	0.5633	Ne^{4+}	0.6080	Na^{4+}	0.6526	Mg^{4+}	0.6971	Al^{4+}	0.7415
Ne^{5+}	0.6530	Mg^{6+}	0.7871	Mg^{5+}	0.7424	Al^{5+}	0.7871	Si^{5+}	0.8316

TABLE 10. ION ENERGIES (RYDBERGS)

		I	II	III
O^+	$E(^2D) - E(^4S)$	0.2718	0.2786	0.2444
	$E(^2P) - E(^4S)$	0.4530	0.4610	0.3688
O^{2+}	$E(^1D) - E(^3P)$	0.2046	0.2058	0.1848
	$E(^1S) - E(^3P)$	0.5116	0.5078	0.3936

I From solutions of Hartree-Fock equations neglecting $\lambda = 2$ terms.

II From solutions of Hartree-Fock equations including $\lambda = 2$ terms (Froese 1967).

III Experiment.

(b) *The exact resonance and distorted wave calculations*

Programs for the e.r. and d.w. calculations were written in Atlas Autocode and run on the University of London Atlas Computer. A typical e.r. run (p -waves only, one ion, three energies) took about 3 min, and a typical d.w. run (one ion, three energies, all partial waves giving significant contributions) took about 2 min. The Fox-Goodwin method was used for evaluation of the y_λ integrals, (2.30), and Weddle's rule was used for the calculation of the definite integrals R_λ , (2.31). As a check on the accuracy of our y_λ and R_λ integration routines, and of adopted step-lengths, we compared our results with those obtained from the program of Froese; in all cases we obtained agreement to at least 5 significant figures. Numerov's method was used for the calculation of radial functions (Hartree 1955, 1957), asymptotic forms of radial functions were determined using the method of Burgess (1963), together with a subroutine provided by Dr G. Peach for the evaluation of Γ functions of complex argument.

The exact resonance equations (2.74) are written

$$(\mathcal{L}_1^{(0)} - k^2) \phi + \eta P = W\phi - 2ty_0(P\phi)P \quad (3.1)$$

and solved by iterating on the right-hand side. At each stage of the iteration η is adjusted in such a way that (2.75) is satisfied (Seaton 1953*b*) and an iteration-variation method is used (Saraph & Seaton 1962). The convergence is found to be very fast, two or three iterations being sufficient in nearly all cases. When allowance is made for energy differences, the matrices ρ^t and L^t in the e.r. approximation are not symmetric but $\rho^K = \rho^t - L^t$ is symmetric. The symmetry of the calculated matrix ρ^K provides a good check on the accuracy of the numerical work, and on the consistency of the approximation.

The e.r. and d.w. programs give print out of various intermediate results and punched-card output of \mathbf{R} matrices. These cards are used as input to various subsequent programs.

(c) *Calculation of collision strengths*

The \mathbf{S} matrix is given by
$$\mathbf{S} = (1 + i\mathbf{R})(1 - i\mathbf{R})^{-1} \quad (3.2)$$

which may be written
$$\mathbf{S} = (1 + i\mathbf{R})^2(1 + \mathbf{R}^2)^{-1}. \quad (3.3)$$

It has already been noted that the elements of \mathbf{R} are sometimes very large, and in some cases it is found that large numerical errors may arise in transforming \mathbf{R} from LS to $J_i j$ coupling. We therefore put $\mathbf{R} = \mathbf{PQ}^{-1}$ where \mathbf{P} and \mathbf{Q} are not large. The exact forms used for \mathbf{P} and \mathbf{Q} will be discussed in a later paper, but it should be noted here that \mathbf{R} is symmetric but that \mathbf{P} and \mathbf{Q} may not be symmetric. Since \mathbf{R} is symmetric, (3.2) may be written

$$\mathbf{S} = (1 + i\mathbf{R})(1 + \tilde{\mathbf{R}}\mathbf{R})^{-1}(1 + i\tilde{\mathbf{R}}) \quad (3.4)$$

Putting $\mathbf{R} = \mathbf{PQ}^{-1} = \tilde{\mathbf{R}} = \tilde{\mathbf{Q}}^{-1}\tilde{\mathbf{P}}$, we obtain

$$\mathbf{S} = (\mathbf{Q} + i\mathbf{P})(\tilde{\mathbf{Q}}\mathbf{Q} + \mathbf{P}\tilde{\mathbf{P}})^{-1}(\tilde{\mathbf{Q}} + i\tilde{\mathbf{P}}). \quad (3.5)$$

This form is convenient for numerical work. The coefficients required for the transformation from LS to $J_i j$ coupling were calculated using programs supplied by the Atomic Physics Group at the Meudon Observatory.

All final calculations of collision strengths were carried out on the I.B.M. 360/65 computer at University College London.

3.2. *Collision strengths in LS coupling*

(a) *Energy values*

It is convenient to take the independent energy variable to be $\epsilon_3 = (k_3/z)^2$. For all ions considered, \mathbf{R} matrices were calculated for $\epsilon_3 = +0.00, 0.05$ and 0.10 , and for some ions additional calculations were made for $\epsilon_3 = 0.25$ and 0.50 .

We introduce the quantity $\epsilon_{23} = \epsilon_2 - \epsilon_3$; then $z^2\epsilon_{23}$ is the energy difference, in rydbergs, between states 2 and 3. Calculations of $\bar{\Omega}(1, 2)$, by means of the Gailitis formula (2.86), were made for $\epsilon_3 = -\epsilon_{23}, -\frac{1}{2}\epsilon_{23}$ and -0.00 , where it should be noted that $\epsilon_3 = -\epsilon_{23}$ corresponds to the threshold for the (1, 2) transition, $\epsilon_2 = +0.00$.

(b) *Partial wave results*

Table 11 gives partial wave results for three typical cases, O^{2+} ($q = 2$), O^+ ($q = 3$) and Ne^{2+} ($q = 4$). In this table we consider only one energy, $\epsilon_3 = +0.00$, and we give e.r. results for the p -waves and d.w. results for all other partial waves. The partial wave expansions are

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE 97

TABLE 11. PARTIAL WAVE CONTRIBUTIONS TO COLLISION STRENGTHS FOR O^{2+} , O^+ AND Ne^{2+} , AND COMPARISON WITH RESULTS OF SEATON (1953*b*, 1955). ALL RESULTS FOR $\epsilon_3 = 0.00$

l	l'	present results			results of Seaton (1953 <i>b</i> , 1955 <i>a</i>)		
		$\Omega(1, 2)$	$\Omega(1, 3)$	$\Omega(2, 3)$	$\Omega(1, 2)$	$\Omega(1, 3)$	$\Omega(2, 3)$
$O^{2+} (q = 2)$							
1	1	1.6644	0.2094	0.0119	1.73	0.195	0.034
2	2	0.7179	0.1250	0.0896	—	—	0.434
3	3	0.0026	0.0002	0.0466	—	—	0.079
4	4	0.0000	0.0000	0.0085	—	—	0.022
$l = l' \geq 5$		0.0000	0.0000	0.0085	—	—	—
0	2	0.0004	0.0000	0.0352	—	—	0.073
2	0	0.0010	0.0000	0.0560	—	—	
1	3	0.0012	0.0000	0.0054	—	—	—
3	1	0.0023	0.0000	0.0426	—	—	—
2	4	0.0004	0.0000	0.0000	—	—	—
4	2	0.0007	0.0000	0.0054	—	—	—
totals		2.3909	0.3346	0.3097	1.73	0.195	0.642
$O^+ (q = 3)$							
1	1	1.3227	0.3925	0.6202	1.4400	0.218	0.595
2	2	0.0998	0.0349	0.4053	0.0170	—	0.827
3	3	0.0001	0.0000	0.0586	0.0032	—	0.146
4	4	0.0000	0.0000	0.0060	—	—	0.043
$l = l' \geq 5$		0.0000	0.0000	0.0000	—	—	—
0	2	0.0044	0.0000	0.0747	0.0032	—	0.290
2	0	0.0036	0.0000	0.3110	0.0032	—	
1	3	0.0003	0.0000	0.0066	—	—	0.017
3	1	0.0002	0.0000	0.1719	—	—	
2	4	0.0001	0.0000	0.0001	—	—	—
4	2	0.0001	0.0000	0.0860	—	—	—
totals		1.4313	0.4274	1.7403	1.467	0.218	1.918
$Ne^{2+} (q = 4)$							
1	1	0.9814	0.1185	0.0123	0.76	0.077	(0.00)*
2	2	0.2864	0.0456	0.0623	—	—	(0.24)*
3	3	0.0006	0.0001	0.0211	—	—	
4	4	0.0000	0.0000	0.0035	—	—	—
$l = l' \geq 5$		0.0000	0.0000	0.0006	—	—	—
0	2	0.0012	0.0000	0.0180	—	—	(0.03)*
2	0	0.0011	0.0000	0.0406	—	—	
1	3	0.0008	0.0000	0.0020	—	—	—
3	1	0.0007	0.0000	0.0226	—	—	—
2	4	0.0001	0.0000	0.0000	—	—	—
4	2	0.0002	0.0000	0.0053	—	—	—
totals		1.2725	0.1642	0.1883	0.76	0.077	(0.27)*

* Values estimated by Seaton (1955) using extrapolation procedures.

seen to converge rapidly for the (1, 2) and (1, 3) transitions, which involve a change of ion spin; for these transitions the p -wave contributions are dominant but the d -wave contributions are also important. The convergence for $\Omega(1, 2)$ is seen to be slower than that for $\Omega(1, 3)$, which is a consequence of the smaller energy difference for the (1, 2) transition. The partial wave expansion is seen to converge much more slowly for $\Omega(2, 3)$; this transition does not involve a spin change and the contributions from the higher-order partial waves are largely determined by quadrupole potential coupling.

(c) Comparison with previous calculations

Table 11 includes a comparison with the earlier results of Seaton (1953*b*, 1955*a*). For the p -waves the present e.r. results agree rather well with the earlier and much cruder, e.r. calculations.

For O^{2+} the earlier results, for the total collision strengths $\Omega(1, 2)$ and $\Omega(1, 3)$ are too small, owing to neglect of contributions from the d -waves. In the earlier work the contributions to $\Omega(2, 3)$ from $l > 1$ were calculated using distorted wave and coulomb wave approximations, neglecting exchange and neglecting energy differences. For O^{2+} neglect of exchange led to the d -wave contribution to $\Omega(2, 3)$ being overestimated, and neglect of energy differences led to the contributions from $l > 2$ being overestimated.

TABLE 12. COMPARISON OF E.R. AND D.W. RESULTS FOR p -WAVE CONTRIBUTIONS TO COLLISION STRENGTHS, AT TWO ENERGIES

ion	ϵ_3	$\Omega^{PP}(1, 2)$		$\Omega^{PP}(1, 3)$		$\Omega^{PP}(2, 3)$	
		e.r.	d.w.	e.r.	d.w.	e.r.	d.w.
N^+	0.0	2.685	1.237	0.304	0.092	0.0301	0.0043
	0.1	2.671	1.435	0.311	0.133	0.0308	0.0067
O^{2+}	0.0	1.664	1.395	0.209	0.180	0.0119	0.0084
	0.1	1.525	1.344	0.202	0.175	0.0101	0.0076
F^{3+}	0.0	1.046	0.956	0.134	0.126	0.0050	0.0040
	0.1	0.870	0.816	0.111	0.105	0.0040	0.0034
Ne^{4+}	0.0	0.690	0.649	0.088	0.084	0.0029	0.0025
	0.1	0.529	0.507	0.066	0.063	0.0030	0.0029
O^+	0.0	1.323	0.543	0.393	0.103	0.620	0.133
	0.1	1.340	0.675	0.409	0.154	0.646	0.192
F^{2+}	0.0	0.961	0.838	0.310	0.276	0.473	0.385
	0.1	0.919	0.840	0.300	0.280	0.452	0.394
Ne^{3+}	0.0	0.666	0.628	0.218	0.212	0.319	0.295
	0.1	0.587	0.562	0.191	0.187	0.277	0.260
Na^{4+}	0.0	0.467	0.447	0.152	0.150	0.218	0.207
	0.1	0.380	0.363	0.122	0.120	0.175	0.168
F^+	0.0	1.23	0.592	0.138	0.030	0.0187	0.0047
	0.1	1.25	0.698	0.143	0.044	0.0197	0.0049
Ne^{2+}	0.0	0.981	0.870	0.118	0.096	0.0123	0.0088
	0.1	0.960	0.882	0.116	0.101	0.0117	0.0092
Na^{3+}	0.0	0.730	0.688	0.089	0.083	0.0068	0.0059
	0.1	0.668	0.634	0.081	0.077	0.0058	0.0052
Mg^{4+}	0.0	0.538	0.518	0.065	0.063	0.0041	0.0037
	0.1	0.459	0.442	0.056	0.053	0.0034	0.0032

(d) Comparison of e.r. and d.w. approximations

Table 12 gives p -wave contributions to the collision strengths, in the e.r. and d.w. approximations, for $\epsilon_3 = +0.00$ and 0.10 . The difference between the e.r. and d.w. results is seen to be large for the singly charged ions, but much smaller for the more highly charged systems. This difference is also seen to decrease as the energy increases, which is what we

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE 99

would expect. The d.w. approximations for $l > 1$ should be much better than the d.w. approximation for $l = 1$.

It is found that the variational corrections \mathbf{L}^l in (2.23), $\rho^K = \rho^l - \mathbf{L}^l$, are reasonably small in all e.r. calculations for $l = 1$, and in all d.w. calculations for $l > 1$, and we therefore conclude that our final results for ρ^K should agree closely with results which would be obtained from exact solutions of the full coupled equations.

The d.w. radial functions may be rather inaccurate for the s -waves. Transitions

$$S_i L_i l \rightarrow S'_i L'_i l' \quad \text{with} \quad S_i L_i \neq S'_i L'_i$$

involve a change in the ion orbital angular momentum, and hence cannot occur if $l = l' = 0$. The contributions from $(l, l') = (0, 2)$ and $(2, 0)$ are small, as can be seen from the results quoted in table 11, and possible inaccuracies in these contributions will not introduce significant errors in the total $S_i L_i \rightarrow S'_i L'_i$ collision strengths.

Further checks on the accuracy of our results will be given in a later paper.

TABLE 13. COLLISION STRENGTHS $\Omega(1, 3)$ AND $\Omega(2, 3)$ AT $\epsilon_3 = 0.00, 0.05$
AND 0.10

ϵ_3	ion	$\Omega(1, 3)$	$\Omega(2, 3)$	ion	$\Omega(1, 3)$	$\Omega(2, 3)$	ion	$\Omega(1, 3)$	$\Omega(2, 3)$
0.00	N ⁺	0.342	0.376	O ⁺	0.428	1.74	F ⁺	0.147	0.193
0.05		0.356	0.389		0.445	1.81		0.152	0.200
0.10		0.369	0.397		0.462	1.87		0.157	0.206
0.00	O ²⁺	0.335	0.310	F ²⁺	0.461	1.71	Ne ²⁺	0.164	0.188
0.05		0.345	0.319		0.483	1.77		0.173	0.194
0.10		0.351	0.326		0.500	1.82		0.180	0.201
0.00	F ³⁺	0.280	0.235	Ne ³⁺	0.427	1.44	Na ³⁺	0.163	0.157
0.05		0.275	0.237		0.431	1.46		0.168	0.161
0.10		0.266	0.238		0.428	1.46		0.170	0.163
0.00	Ne ⁴⁺	0.218	0.185	Na ⁴⁺	0.359	1.17	Mg ⁴⁺	0.146	0.129
0.05		0.203	0.187		0.346	1.16		0.144	0.131
0.10		0.186	0.186		0.327	1.13		0.141	0.133
0.00	Mg ⁶⁺	0.128	0.123	Mg ⁵⁺	0.289	0.942	Al ⁵⁺	0.123	0.107
0.05		0.110	0.123		0.266	0.916		0.116	0.108
0.10		0.094	0.122		0.241	0.882		0.109	0.109

(e) *Energy variation of the collision strengths*

Table 13 gives values of $\Omega(1, 3)$ and $\Omega(2, 3)$ for $\epsilon_3 = +0.00, 0.05$ and 0.10 .

For $\Omega(1, 2)$ we have to consider energies such that $\epsilon_3 < 0$ but $\epsilon_2 \geq 0$. Table 14 gives results for $\Omega(1, 2)$ at energies $\epsilon_3 = -\epsilon_{23}, -\frac{1}{2}\epsilon_{23}$ and -0.00 , calculated by the Gailitis formula (2.86), together with results for $\epsilon_3 = +0.00, 0.05$ and 0.10 . The discontinuity at $\epsilon_3 = 0.00$ is fairly small, which is a consequence of $\Omega(1, 3)$ being small compared with $\Omega(1, 2)$. As a check on the numerical work, it was verified that numerical integration over resonances gave results in close agreement with those obtained from the Gailitis formula.

(f) *Iso-electronic sequences*

It may be shown that, as the charge z tends to infinity, $z^2\Omega$ remains finite. In table 15 we give values of $(z^2\Omega)_\infty = \lim_{z \rightarrow \infty} (z^2\Omega)$.

TABLE 14. ENERGY VARIATION OF $\Omega(1, 2)$ (NOTE THAT $\epsilon_3 = -\epsilon_{23}$ CORRESPONDS TO $\epsilon_2 = 0.00$)

ϵ_3	$\Omega(1, 2)$				
	N ⁺	O ²⁺	F ³⁺	Ne ⁴⁺	Mg ⁶⁺
$-\epsilon_{23}$	2.81	2.45	1.95	1.49	0.866
$-\frac{1}{2}\epsilon_{23}$	2.99	2.48	1.93	1.46	0.850
-0.00	3.15	2.50	1.91	1.43	0.833
+0.00	3.05	2.39	1.83	1.38	0.800
0.05	3.10	2.40	1.76	1.28	0.700
0.10	3.14	2.39	1.69	1.17	0.609
	O ⁺	F ²⁺	Ne ³⁺	Na ⁴⁺	Mg ⁵⁺
$-\epsilon_{23}$	1.36	1.33	1.14	0.919	0.717
$-\frac{1}{2}\epsilon_{23}$	1.47	1.36	1.14	0.913	0.710
-0.00	1.55	1.38	1.14	0.905	0.703
+0.00	1.43	1.25	1.04	0.836	0.652
0.05	1.46	1.28	1.03	0.799	0.604
0.10	1.48	1.29	1.01	0.755	0.555
	F ⁺	Ne ²⁺	Na ³⁺	Mg ⁴⁺	Al ⁵⁺
$-\epsilon_{23}$	1.16	1.24	1.17	1.02	0.844
$-\frac{1}{2}\epsilon_{23}$	1.27	1.29	1.18	1.02	0.835
-0.00	1.37	1.33	1.20	1.02	0.826
+0.00	1.34	1.27	1.14	0.973	0.792
0.05	1.36	1.31	1.15	0.952	0.750
0.10	1.39	1.34	1.15	0.919	0.701

TABLE 15. VALUES OF $(z^2\Omega)_\infty = \lim_{z \rightarrow \infty} (z^2\Omega)$, FOR $\epsilon_3 = 0.00$

	$(z^2\Omega(1, 2))_\infty$	$(z^2\Omega(1, 3))_\infty$	$(z^2\Omega(2, 3))_\infty$
$q = 2$ and 4	42.8	5.83	12.5
$q = 3$	31.6	11.7	66.9

TABLE 16. PARTIAL WAVE CONTRIBUTIONS TO COLLISION STRENGTHS $\Omega(^2P_{\frac{1}{2}}, ^2P_{\frac{3}{2}})$ IN C⁺ ($q = 1$) AND Ne⁺ ($q = 5$) FOR $\epsilon = 0.00$

l	l'	$\Omega(^2P_{\frac{1}{2}}, ^2P_{\frac{3}{2}})$	
		C ⁺	Ne ⁺
1	1	1.0342	0.18381
2	2	0.3228	0.05095
0	2		
2	0		
0	0		
1	3	0.0559	0.00675
3	1		
3	3		
2	4	0.0001	0.00000
4	2		
4	4	0.0095	0.00139
$l = l' \geq 5$		0.0090	0.00133
totals		1.4315	0.24423

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE 101

TABLE 17. COLLISION STRENGTHS $\Omega(^2P_{\frac{1}{2}}, ^2P_{\frac{3}{2}})$ FOR $q = 1$ AND $q = 5$

ϵ \ ion	$q = 1$				
	C ⁺	N ²⁺	O ³⁺	F ⁴⁺	Ne ⁵⁺
0.00	1.432	1.097	0.810	0.578	0.433
0.05	1.462	1.097	0.773	0.533	0.387
0.10	1.487	1.088	0.733	0.490	0.347

ϵ \ ion	$q = 5$				
	Ne ⁺	Na ²⁺	Mg ³⁺	Al ⁴⁺	Si ⁵⁺
0.00	0.244	0.300	0.300	0.277	0.242
0.05	0.255	0.313	0.309	0.279	0.236
0.10	0.265	0.324	0.317	0.278	0.228

For $q = 1$ and 5, at $\epsilon = 0.00$, $(z^2\Omega)_{\infty} = 18.6$.

TABLE 18. PARTIAL WAVE CONTRIBUTIONS TO COLLISION STRENGTHS

 $\Omega(^3P_J, ^3P_{J'})$ IN O²⁺, FOR $\epsilon_3 = 0.00$

l	l'	$\Omega(^3P_0, ^3P_1)$	$\Omega(^3P_0, ^3P_2)$	$\Omega(^3P_1, ^3P_2)$
1	1	0.1934	0.0863	0.4361
1	3	0.0012	0.0291	0.0670
3	1			
3	3			
0	0	0.1812	0.0878	0.4235
0	2			
2	0			
2	2			
$l = l' \geq 4$		0.0000	0.0094	0.0211
totals		0.3758	0.2126	0.9477

TABLE 19. COLLISION STRENGTHS $\Omega(^3P_J, ^3P_{J'})$ FOR $q = 2$ AND 4

ϵ_3	ion	$\Omega(^3P_0, ^3P_1)$	$\Omega(^3P_0, ^3P_2)$	$\Omega(^3P_1, ^3P_2)$	ion	$\Omega(^3P_0, ^3P_1)$	$\Omega(^3P_0, ^3P_2)$	$\Omega(^3P_1, ^3P_2)$
0.00	N ⁺	0.401	0.279	1.128	F ⁺	0.1735	0.1432	0.539
0.05		0.413	0.281	1.474		0.1780	0.1457	0.551
0.10		0.424	0.282	1.164		0.1824	0.1480	0.561
0.00	O ²⁺	0.376	0.213	0.948	Ne ²⁺	0.1845	0.1314	0.527
0.05		0.385	0.210	0.954		0.1927	0.1284	0.540
0.10		0.391	0.207	0.954		0.1997	0.1337	0.551
0.00	F ³⁺	0.219	0.165	0.645	Na ³⁺	0.1769	0.1107	0.471
0.05		0.211	0.160	0.623		0.1813	0.1094	0.473
0.10		0.201	0.154	0.598		0.1832	0.1076	0.472
0.00	Ne ⁴⁺	0.244	0.122	0.578	Mg ⁴⁺	0.1558	0.0908	0.400
0.05		0.230	0.114	0.543		0.1544	0.0874	0.390
0.10		0.215	0.107	0.507		0.1513	0.0843	0.380
0.00	$(z^2\Omega)_{\infty}$ for $q = 2$ and 4	7.52	5.91	22.7				

TABLE 20. PARTIAL WAVE CONTRIBUTIONS TO COLLISION STRENGTHS FOR TRANSITIONS BETWEEN FINE STRUCTURE LEVELS IN O^+ , $\epsilon_3 = 0.00$

l	l'	$\Omega(^2D_{3/2}, ^2D_{5/2})$	$\Omega(^2D_{3/2}, ^2P_{1/2})$	$\Omega(^2D_{3/2}, ^2P_{3/2})$	$\Omega(^2D_{5/2}, ^2P_{1/2})$	$\Omega(^2D_{5/2}, ^2P_{3/2})$	$\Omega(^2P_{1/2}, ^2P_{3/2})$
1	1	0.8209	0.0585	0.1896	0.1482	0.2239	0.2482
1	3	0.0005	0.0474	0.0474	0.0316	0.1106	0.0001
3	1						
3	3						
0	0	0.0723	0.1545	0.1622	0.1094	0.3655	0.0148
0	2						
2	0						
2	2						
$l' \geq 4$		0.0000	0.0186	0.0186	0.0124	0.0432	0.0000
	totals	0.8937	0.2790	0.4178	0.3016	0.7432	0.2631

TABLE 21. COLLISION STRENGTHS FOR TRANSITIONS BETWEEN FINE STRUCTURE STATES IN IONS WITH $q = 3$

ϵ_3	ion	$\Omega(^2D_{3/2}, ^2D_{5/2})$	$\Omega(^2D_{3/2}, ^2P_{1/2})$	$\Omega(^2D_{3/2}, ^2P_{3/2})$	$\Omega(^2D_{5/2}, ^2P_{1/2})$	$\Omega(^2D_{5/2}, ^2P_{3/2})$	$\Omega(^2P_{1/2}, ^2P_{3/2})$
0.00	O^+	0.894	0.279	0.418	0.302	0.743	0.263
0.05		0.918	0.290	0.435	0.314	0.773	0.276
0.10		0.941	0.302	0.451	0.325	0.803	0.288
0.00	F^{2+}	0.889	0.282	0.403	0.289	0.732	0.372
0.05		0.917	0.281	0.427	0.309	0.754	0.358
0.10		0.941	0.284	0.444	0.323	0.770	0.357
0.00	Ne^{3+}	0.817	0.234	0.342	0.246	0.619	0.446
0.05		0.806	0.225	0.359	0.262	0.615	0.357
0.10		0.796	0.222	0.363	0.265	0.612	0.326
0.00	Na^{4+}	0.696	0.190	0.279	0.201	0.502	0.438
0.05		0.640	0.175	0.287	0.210	0.484	0.294
0.10		0.612	0.170	0.281	0.206	0.473	0.252
0.00	$(z^2\Omega)_\infty$	24.8	13.4	17.3	12.2	33.9	9.39

In the limit of z large our results will be in error due to neglect of spin-dependent terms in the Hamiltonian, and other relativistic effects. Even as solutions of the non-relativistic problem, our results may be appreciably in error in this limit. In the near threshold region in which we are interested, further resonances can arise from coupling to other closed channels, such as those involving configurations $2s2p^{q+1}$. From the Gailitis formula it may be seen that, even in the limit of z large, the collision strengths averaged over these resonances may be different from the collision strengths calculated neglecting the closed channels.

3.3. Transitions between fine structure levels

(a) Configurations $2p$ and $2p^5$

The configurations $2p$ and $2p^5$ contain a single 2P term. Table 16 gives partial wave contributions to $\Omega(^2P_{1/2}, ^2P_{3/2})$ for C^+ and Ne^+ , calculated using the e.r. approximation for the p -waves and the d.w. approximation for all other partial waves. Table 17 gives total collision strengths $\Omega(^2P_{1/2}, ^2P_{3/2})$ for ions in configurations $2p$ and $2p^5$.

(b) Configurations $2p^2$, $2p^3$ and $2p^4$

Using equation (2.14) we obtain

$$\Omega(^1S, ^3P_J) = \frac{1}{8}(2J+1) \Omega(^1S, ^3P); \quad \Omega(^1D, ^3P_J) = \frac{1}{8}(2J+1) \Omega(^1D, ^3P) \quad (3.6)$$

for ions in configurations $2p^2$ and $2p^4$, and

$$\Omega(^4S, ^2D_J) = \frac{1}{10}(2J+1) \Omega(^4S, ^2D); \quad \Omega(^4S, ^2P_J) = \frac{1}{6}(2J+1) \Omega(^4S, ^2P) \quad (3.7)$$

for ions in configurations $2p^3$. These collision strengths may therefore be obtained from the results given in tables 13 and 14.

Table 18 gives partial wave contributions to the collision strengths $\Omega(^3P_J, ^3P_{J'})$ for O^{2+} . The transition $(J, J') = (0, 1)$ differs from the other two transitions in that it has a zero quadrupole moment. In consequence the partial wave expansions for $(J, J') = (0, 1)$ converge much more rapidly. Table 19 gives total collision strengths $\Omega(^3P_J, ^3P_{J'})$ for ions in configurations $2p^2$ and $2p^4$. Transitions of the type $^3P_J l \rightarrow ^3P_{J'} l'$, do not involve a change in the ion orbital angular momentum, and can occur for $l = l' = 0$ if $J' = J \pm 1$. It is found that transitions

$$^3P_{0s} \rightarrow ^3P_{1s} \quad \text{and} \quad ^3P_{1s} \rightarrow ^3P_{2s},$$

for which the d.w. method may not be too accurate, make significant contributions to the total $^3P_0 \rightarrow ^3P_1$ and $^3P_1 \rightarrow ^3P_2$ collision strengths.

Table 20 gives partial wave contributions to $\Omega(^2D_J, ^2D_{J'})$, $\Omega(^2D_J, ^2P_{J'})$ and $\Omega(^2P_J, ^2P_{J'})$ in O^+ , and table 21 gives total collision strengths for these transitions in $2p^3$ ions. Quadrupole moments occur only in the $^2D_J \rightarrow ^2P_{J'}$ transitions. Further results for $\Omega(^2D_J, ^2D_{J'})$ at energies $\epsilon_3 < 0$ will be given in a later paper.

We are indebted to our collaborators in this project, Dr S. J. Czyzak, Mr T. K. Krueger and Dr P. de A. P. Martins, for many helpful discussions, and to Dr Martins for assistance with the final production work.

The work has been supported by grants from the Science Research Council and from the Culham Laboratory of the Atomic Energy Research Establishment.

Note added in proof (October 1968)

(i) K. Smith, M. J. Conneely and L. A. Morgan (private communication) and R. J. W. Henry, P. G. Burke and A-L. Sinfailam (private communication) have drawn attention to an error in the formulation of the problem of electron collisions with ions in configurations $1s^2 2s^2 2p^q$ given by Smith, Henry & Burke (1966). When this error is corrected, their formulation should be identical with ours. These authors have calculated collision strengths from exact solutions of the coupled equations. Our results agree with those of Smith, Conneely & Morgan for N^+ and O^{2+} to within 10%. There are slightly larger differences between our results and those of Henry, Burke & Sinfailam for N^+ , O^+ and O^{2+} , probably due to these authors having used experimental energy differences in solving the radial equations.

(ii) Recent work by W. Eissner, H. Nussbaumer, H. E. Saraph & M. J. Seaton (to

be published) shows that allowance for coupling between the configurations $2s^22p^2$ and $2s2p^3$ gives rise to near-threshold resonances in the collision strengths for excitation of the $2s^22p^2$ terms in O^{2+} .

(iii) Small differences between the present results for $2p^3$ ions and those published previously (Czyzak *et al.* 1967) are due to the correction of a minor error in one of the computer programs.

Note added in proof 30 December 1968

The page proofs of tables 5 to 8 have been checked by means of a computer (December, 1968). Working directly from the proofs, the algebraic expressions given in these tables have been punched as Fortran statements, and a computer program has been written to calculate numerical values from these expressions and to compare with values obtained using the program of Drs W. Eissner and H. Nussbaumer. We are indebted to Dr Eissner for his help with this work. The computer checks revealed several errors which had not been detected previously. We may hope that tables 5 to 8, as published, are completely free of error.

REFERENCES

- Aller, L. H. & Liller, W. 1968 *Nebulae and interstellar matter* (ed. B. M. Middlehurst & L. H. Aller), pp. 483–574. Chicago University Press.
- Aller, L. H., Ufford, C. W. & Van Vleck, J. H. 1949 *Astrophys. J.* **109**, 42.
- Ambartsumian, V. A. 1933 *Tsirkulyary Glavnoi Astronomicheskoi Observatorii* **6**, 10.
- Bates, D. R., Fundaminsky, A. & Massey, H. S. W. 1950 *Phil. Trans. A* **243**, 93.
- Bely, O., Moores, D. E. & Seaton, M. J. 1963 *Atomic Collision Processes* (ed. M. R. C. McDowell). Amsterdam: North-Holland.
- Bowen, I. S. 1928 *Astrophys. J.* **67**, 1.
- Burgess, A. 1963 *Proc. Phys. Soc.* **81**, 442–52.
- Condon, E. U. & Shortley, G. H. 1935 *Theory of atomic spectra*. Cambridge University Press.
- Czyzak, S. J. & Krueger, T. K. 1967 *Proc. Phys. Soc.* **90**, 623–7.
- Czyzak, S. J., Krueger, T. K., Saraph, H. E. & Shemming, J. 1967 *Proc. Phys. Soc.* **92**, 1146–7.
- Czyzak, S. J., Krueger, T. K., Martins, P. de A. P., Saraph, H. E., Seaton, M. J. & Shemming, J. 1968 *Planetary nebulae* (ed. D. E. Osterbrock & C. R. O'Dell), pp. 138–42. Dordrecht-Holland: D. Reidel.
- Edmonds, A. R. 1957 *Angular momentum in quantum mechanics*. Princeton University Press.
- Frocse, C., 1967 *Proc. Phys. Soc.* **90**, 39–42.
- Garstang, R. H. 1968 *Planetary nebulae* (ed. D. E. Osterbrock & C. R. O'Dell), pp. 143–52. Dordrecht-Holland: D. Reidel.
- Gailitis, M. 1963 *Soviet Phys.—JETP*, **17**, 1328–32.
- Godfredsen, E. 1966 *Astrophys. J.* **145**, 308–32.
- Hartree, D. R. 1955 *Numerical analysis*. Oxford University Press.
- Hartree, D. R. 1957 *The calculation of atomic structures*. New York: Wiley.
- Hartree, D. R., Hartree, W. & Swirles, B. 1939 *Phil. Trans. A* **238**, 229–47.
- Hebb, M. H. & Menzel, D. H. 1940 *Astrophys. J.* **92**, 408–23.
- Huggins, W. 1864 *Phil. Trans.* **154**, 437–44.
- Kohn W. 1948 *Phys. Rev.* **74**, 1763–72.
- Menzel, D. H., Aller, L. H. & Hebb, M. H. 1941 *Astrophys. J.* **93**, 230–5.
- Percival, I. C. & Seaton, M. J. 1957 *Proc. Camb. Phil. Soc.* **53**, 654–62.
- Salmona, A. & Seaton, M. J. 1961 *Proc. Phys. Soc.* **77**, 617–29.
- Saraph, H. E. & Seaton, M. J. 1962 *Proc. Phys. Soc.* **80**, 1057–66.

EXCITATION OF FORBIDDEN LINES IN GASEOUS NEBULAE 105

- Saraph, H. E., Seaton, M. J. & Shemming, J. 1966 *Proc. Phys. Soc.* **89**, 27–34.
- Seaton, M. J. 1953 *a Phil. Trans. A* **245**, 469–99.
- Seaton, M. J. 1953 *b Proc. Roy. Soc. A* **218**, 400–416.
- Seaton, M. J. 1955 *a Proc. Roy. Soc. A* **231**, 37–52.
- Seaton, M. J. 1955 *b The air glow and the aurorae* (ed. E. B. Armstrong & A. Dalgarno), pp. 289–301. London and New York: Pergamon Press.
- Seaton, M. J. 1958 *Rev. Mod. Phys.* **30**, 979–89.
- Seaton, M. J. 1962 *Atomic and molecular processes* (ed. D. R. Bates). London and New York: Academic Press.
- Seaton, M. J. 1966 *Proc. Phys. Soc.* **88**, 801–14.
- Seaton, M. J. 1967 *Proc. Phys. Soc.* **89**, 469–70.
- Seaton, M. J. 1968 *a Advances in atomic and molecular physics* (ed. D. R. Bates & I. Esterman), vol. iv. London and New York: Academic Press.
- Seaton, M. J. 1968 *b Planetary nebulae* (ed. D. E. Osterbrock & C. R. O'Dell), pp. 129–37. Dordrecht-Holland: D. Reidel.
- Seaton, M. J. & Osterbrock, D. E. 1957 *Astrophys. J.* **125**, 66–83.
- Shemming, J. 1965 Thesis, University of London.
- Slater, J. C. 1960 *Quantum theory of atomic structure*, vol. II, pp. 288–291. New York: McGraw Hill.
- Smith, K., Henry, R. J. W. & Burke, P. G. 1966 *Phys. Rev.* **147**, 21.
- Yamanouchi, T. & Amemiya, A. 1946 *J. Phys. Soc. Japan* **1**, 18–23.
- Yamanouchi, T., Inui, I. & Amemiya, A. 1940 *Proc. Phys. Math. Soc. Japan* **22**, 847.