On the Excitation of O_{III}-ion in $2p^2$-Configuration by the Electron Impact

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Summary

§ 1. In connection with the problem, discussed in the previous paper[1] on the gas temperature of planetary nebulae, we shall state in this paper the calculation of the effective cross-section of the oxygen ion O_{III} for impact excitation by free electron[2].

In Part I, we construct the wave equation for the system consisting of a O_{III} ion and of a free electron; and give its solution according to Born's approximation. In Part II, the angular part of the function is integrated. The integration of the radial part is given in Part III. And finally in part IV, the effective cross-section of O_{III} for collisional excitation is given.

I. Formulation

§ 2. *Wave equation.* O_{III} consists of two saturated shells, 1s and 2s, each having two electrons and of an unsaturated one, 2p, with two electrons. We shall denote in the following the first four by I, II, III, IV, which will be often represented by latin letters i, j etc.; whereas the last two by 1 and 2 and colliding electron by 3.

The Schrödinger equation for the wave function ϕ, which describes the physical system consisting of an O_{III} ion and of a colliding electron is

$$[\sum \nabla_i^2 + \nabla_1^2 + \nabla_2^2 + \nabla_3^2 - \frac{8\pi m}{h}(E-U)]\phi = 0, \tag{2.1}$$

where the potential U is given by

$$U = V + V_0, \tag{2.2}$$

where

1. These memoirs, **22** (1939) 249.

2. Recenly, details of the calculatian of the same problem treated by Malcolm H. Hebb and Donald H. Menzel were published in Ap. J. **92** (1940) 408.

$$V\equiv\varepsilon^2\left(\sum_i\frac{1}{r_{i3}}+\frac{1}{r_{13}}+\frac{1}{r_{23}}-\frac{8}{r_3}\right) \tag{2.3}$$

represents the part of the potential which comes from the interaction between the colliding electron and the atom, and

$$V_0=\varepsilon^2\left\{\sum_{i,j}\frac{1}{r_{ij}}+\sum_i\left(\frac{1}{r_{i1}}+\frac{1}{r_{i2}}-\frac{8}{r_i}\right)-8\left(\frac{1}{r_1}+\frac{1}{r_2}\right)\right\} \tag{2.4}$$

the potential of the undisturbed atom; ε being the elementary charge, r_{ab} the mutual distance between any two electrons a and b and r_a that of any electron a from the nucleus.

§ 3. *Direct Excitation.* As a first approximation, atomic electrons satisfy the wave equation of the undisturbed atom:

$$\left(\sum_i\nabla_i^2+\nabla_1^2+\nabla_2^2\right)\psi(\boldsymbol{r}_1, \boldsymbol{r}_2;\ (\boldsymbol{r}_i))+\frac{8\pi^2m}{h}$$
$$\times(E-V_0)\,\psi(\boldsymbol{r}_1, \boldsymbol{r}_2;\ (\boldsymbol{r}_i))=0, \tag{3.1}$$

where heavy letters mean vectors as usual and $(\boldsymbol{r}_i)$ stands for $\boldsymbol{r}_{\mathrm{I}}, \boldsymbol{r}_{\mathrm{II}}, \boldsymbol{r}_{\mathrm{III}}, \boldsymbol{r}_{\mathrm{IV}}$, for simplicity's sake. Now, we denote by ψ_n a solution of this equation, viz., an eigen-function corresponding to state n, of which energy is E_n. In the following, throughout this paper, we shall use n for the initial state and n' for the excited final state.

In order to see the probability of direct excitation, by which process the impinging electron 3 is scattered inelastically and the atomic electrons are left in the excited state n', we have to determine the coefficient $F_{nn'}(\boldsymbol{r}_3)$ of $\psi_{n'}(\boldsymbol{r}_1, \boldsymbol{r}_2;\ (\boldsymbol{r}_i))$ in the expansion of ϕ:

$$\phi=\left(\sum_{n'}+\int dn'\right)\psi_{n'}(\boldsymbol{r}_1, \boldsymbol{r}_2;\ (\boldsymbol{r}_i))F_{nn'}(\boldsymbol{r}_3). \tag{3.2}$$

Summation and integration in (3.2) are to be referred to all the discrete and the continuous states n'. For large r, $F_{nn'}$ must have the asymptotic form:

$$F_{nn'}(\boldsymbol{r})\sim e^{ikz}+\frac{e^{ikr}}{r}f_{nn}(\theta)\qquad\text{for } n=n', \tag{3.3}$$
$$\sim\qquad\frac{e^{ik'r}}{r}f_{nn'}(\theta)\qquad\text{otherwise,}$$

where

$$k\equiv k_{nn}\equiv\frac{2\pi m}{h}v \tag{3.4}$$

$$k'^2\equiv k_{nn'}^2\equiv\frac{8\pi^2m}{h^2}\left(\frac{1}{2}mv^2-|E_n-E_{n'}|\right), \tag{3.5}$$

and e^{ikz} means the wave of the incident electron of velocity v along z-axis and of unit density, and θ means the angle of scattering. Inserting into the Schrödinger equation the expressions (2.2–4) and (3.2), and multiplying it by $\psi_{n'}^*(\boldsymbol{r}_1, \boldsymbol{r}_2\,;\,(\boldsymbol{r}_i))$ and then integrating it over the whole space of $\boldsymbol{r}_1, \boldsymbol{r}_2$ and $(\boldsymbol{r}_i)$, we get[1]

$$(\nabla_3^2+k'^2)F_{nn'}(\boldsymbol{r}_3)=\frac{8\pi m}{h^2}\int\psi_{n'}^*(\boldsymbol{r}_1, \boldsymbol{r}_2\,;\,(\boldsymbol{r}_i))V\phi dv_1 dv_2(dv_i). \quad (3.6)$$

§ 4. *Exchange Excitation.* In order to see the probability of exchange excitation, by which one of the atomic electrons, e. g. 1, is expelled and the impinging electron 3 is captured by the ion, we express ϕ in another form, alternative with (3.2):

$$\phi=\Big(\sum_{n'}+\int dn'\Big)\psi_{n'}(\boldsymbol{r}_3, \boldsymbol{r}_2\,;\,(\boldsymbol{r}_i))G_{nn'}(\boldsymbol{r}_1), \quad (4.1)$$

with the assumption that $G_{nn'}$ has an asymptotic form:

$$G_{nn'}(\boldsymbol{r})\sim\frac{e^{ik'r}}{r}g_{nn'}(\theta) \qquad \text{for large } r. \quad (4.2)$$

Then, in the same way as in § 3, we obtain the equation for $G_{nn'}$:

$$(\nabla_1^2+k'^2)G_{nn'}(\boldsymbol{r}_1)=\frac{8\pi m}{h^2}\int\psi_{n'}^*(\boldsymbol{r}_3, \boldsymbol{r}_2\,;\,(\boldsymbol{r}_i))V'\phi dv_3 dv_2(dv_i), \quad (4.3)$$

where

$$V'\equiv\varepsilon^2\Big(\sum_i\frac{1}{r_{1i}}+\frac{1}{r_{12}}+\frac{1}{r_{13}}-\frac{8}{r_1}\Big). \quad (4.4)$$

The exchange effect of higher order has been neglected, which is connected with electron of saturated shells, 1s and 2s.

§ 5. Equations (3.6) and (4.3) determine $F_{nn'}$ and $G_{nn'}$. We shall follow Born's procedure of approximation taking for ϕ in the second side of the equations the wave function of the configuration of the system before collision, neglecting all the interactions between electron waves and the ionic field:[2]

$$\phi=\psi_n(\boldsymbol{r}_1. \boldsymbol{r}_2\,;\,(\boldsymbol{r}_i))e^{ik\boldsymbol{n}_0\boldsymbol{r}_3}, \quad (5.1)$$

where $\boldsymbol{n}_0$ is the unit vector in the direction of the positive z-axis. Then by inserting (5.1) into (3.6) and (4.5) and solving, we get

$$F_{nn'}(\boldsymbol{r})\sim\frac{e^{ik'r}}{r}f_{nn'}(\theta) \quad (5.2)$$

$$G_{nn'}(\boldsymbol{r})\sim\frac{e^{ik'r}}{r}g_{nn'}(\theta) \quad (5.3)$$

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1. We shall spare with the spin coordinate, as it can easily be seen when it is necessary to consider of.

2. Hebb (loc. cit.) takes the wave function distorted by the ionic field for the colliding electron insteaed of the plane wave approximation. The final result is largely different from ours. It seems that the crosssection is much affected by the starting assumption. For slow collision, plane wave approximation has no theoretical warrant. For distorted wave, perturbing term $V_{nn'}$ becomes very large for small k'.

with

$$f_{nn'}(\theta)=\frac{-1}{2\pi a_0}\int e^{i(k\boldsymbol{n}_0-k'\boldsymbol{n})\boldsymbol{r}_3}\left(\sum_i\frac{1}{r_{3i}}+\frac{1}{r_{13}}+\frac{1}{r_{23}}-\frac{8}{r_3}\right)$$

$$\times\psi_n(\boldsymbol{r}_1,\boldsymbol{r}_2;(\boldsymbol{r}_i))\psi^*_{n'}(\boldsymbol{r}_1,\boldsymbol{r}_2;(\boldsymbol{r}_i))dv_1dv_2(dv_i)dv_3 \qquad (5.4)$$

$$g_{nn'}(\theta)=\frac{-1}{2\pi a_0}\int e^{i(k\boldsymbol{n}_0\boldsymbol{r}_3-k'\boldsymbol{n}\boldsymbol{r}_1)}\left(\sum_i\frac{1}{r_{1i}}+\frac{1}{r_{12}}+\frac{1}{r_{13}}-\frac{8}{r_2}\right)$$

$$\times\psi_n(\boldsymbol{r}_1,\boldsymbol{r}_2;(\boldsymbol{r}_i))\psi^*_{n'}(\boldsymbol{r}_3,\boldsymbol{r}_2;(\boldsymbol{r}_i))dv_3dv_2(dv_i)dv_1, \qquad (5.5)$$

where $\boldsymbol{n}$ is the unit vector in the direction of scattering $\boldsymbol{r}$, and a_0 the Bohr's radius of hydrogen.

§ 6. *f-term.* The full expression of this term has been given by (5.4), in which the contribution from $\frac{8}{r_3}$ and $\sum_i\frac{1}{r_{3i}}$ vanishes. Thus only the contributions from $\frac{1}{r_{13}}$ and $\frac{1}{r_{23}}$ remain in (5.4).

Integrating them with respect to v_3, we get

$$f_{nn'}(\theta)=\frac{-1}{2a_0K'^2}\int\left(\sum_{\alpha=1,2}e^{i(k\boldsymbol{n}_0-k'\boldsymbol{n})\boldsymbol{r}_\alpha}\right)$$

$$\times\psi_n(\boldsymbol{r}_1,\boldsymbol{r}_2;(\boldsymbol{r}_i))\psi^*_{n'}(\boldsymbol{r}_1,\boldsymbol{r}_2;(\boldsymbol{r}_i))dv_1dv_2(dv_i) \qquad (6.1)$$

$$K'^2=|k\boldsymbol{n}_0-k'\boldsymbol{n}|^2. \qquad (6.2)$$

According to our approximation (§ 4), $\psi_n(\boldsymbol{r}_1,\boldsymbol{r}_2;(\boldsymbol{r}_i))$ will be of the form:

$$\psi_n(\boldsymbol{r}_1,\boldsymbol{r}_2;(\boldsymbol{r}_i))=\psi_{1s}(\boldsymbol{r}_{\rm I})\psi_{1s}(\boldsymbol{r}_{\rm II})\psi_{2s}(\boldsymbol{r}_{\rm III})\psi_{2s}(\boldsymbol{r}_{\rm IV})\Phi_n(\boldsymbol{r}_1,\boldsymbol{r}_2), \qquad (6.3)$$

where $\Phi(\boldsymbol{r}_1,\boldsymbol{r}_2)$ is the wave function of two 2p-electrons, and antisymmetric with respect to them. Their radial parts must be of the same form, so that $\Phi_n(\boldsymbol{r}_1,\boldsymbol{r}_2)$ can be written as

$$\Phi_n(\boldsymbol{r}_1,\boldsymbol{r}_2)=\frac{R(r_1)}{r_1}\frac{R(r^2)}{r_2}\Psi_n(\boldsymbol{n}_1,\boldsymbol{n}_2), \qquad (6.4)$$

Ψ_n being the angular part, and n_1 and n_2 are the unit vectors in the directions $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ respectively. Thus (6.1) is reduced to

$$f_{nn'}(\theta)=\frac{-1}{2a_0K'^2}\iint_0^\infty R^2(r_1)dr_1R^2(r_2)dr_2\int(\sum_\alpha e^{i(k\boldsymbol{n}_0-k'\boldsymbol{n})\boldsymbol{r}_\alpha})$$

$$\times\Psi_n(\boldsymbol{n}_1,\boldsymbol{n}_2)\Psi^*_{n'}(\boldsymbol{n}_1,\boldsymbol{n}_2)\sin\theta_1\sin\theta_2d\theta_1d\theta_2d\phi_1d\phi_2. \qquad (6.5)$$

Taking the positive z-axis in the direction of $\boldsymbol{n}_0$, and making use of the polar coordinate, the exponent in (6.5) becomes

$$(k\boldsymbol{n}_0-k'\boldsymbol{n})\boldsymbol{r}_\alpha=r_\alpha(k\cos\theta_\alpha-k'\cos\theta_\alpha\cos\theta-k'\sin\theta_\alpha\sin\phi_\alpha\sin\theta). \qquad (6.6)$$

§ 7. *g-term.* The expression of this term is given by (5.5). Contributions from terms $\sum_i\frac{1}{r_{1i}}$, $\frac{8}{r_1}$ and $\frac{1}{r_{12}}$ are to vanish, and we have

$$g_{mn'}(\theta)=\frac{-1}{2\pi a_0}\int e^{i(k\boldsymbol{n}_0\boldsymbol{r}_3-k'\boldsymbol{n}\boldsymbol{r}_1)}\frac{1}{r_{13}}$$
$$\times\psi_n(\boldsymbol{r}_1,\boldsymbol{r}_2;(\boldsymbol{r}_i))\psi^*_{n'}(\boldsymbol{r}_3,\boldsymbol{r}_2;(\boldsymbol{r}_i))dv_3dv_2(dv_i)dv_1, \quad (7.1)$$

or expanding $\frac{1}{r_{13}}$ by Legendre functions, we obtain

$$g_{mn'}(\theta)=\frac{-1}{2\pi a_0}\iiint_0^\infty R(r_1)r_1dr_1R(r_3)r_3dr_3R^2(r_2)dr_2\times$$
$$\times\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}\int\Psi^*_{n'}(\boldsymbol{n}_3,\boldsymbol{n}_2)\Psi_n(\boldsymbol{n}_1,\boldsymbol{n}_2)\gamma_\alpha\frac{(\alpha-|\beta|)!}{(\alpha+|\beta|)!}\times$$
$$\times P_\alpha^{|\beta|}(\cos\theta_1)P_\alpha^{|\beta|}(\cos\theta_3)e^{i(\phi_1-\phi_3)}\times$$
$$\times e^{i(k\boldsymbol{n}_0\boldsymbol{r}_3-k'\boldsymbol{n}\boldsymbol{r}_1)}\sin\theta_1\sin\theta_3d\theta_1d\theta_3d\phi_1d\phi_3\sin\theta_2d\theta_2d\phi_2, \quad (7.2)$$

with

$$k\boldsymbol{n}_0\boldsymbol{r}_3-k'\boldsymbol{n}\boldsymbol{r}_1=kr_3\cos\theta_3-k'r_1(\mathrm{sos}\,\theta_1\,\mathrm{sos}\,\theta+\sin\theta_1\sin\phi_1\sin\theta) \quad (7.3)$$

$$\gamma_\alpha\equiv\frac{r_1^\alpha}{r_3^{\alpha+1}}\ \text{or}\ \frac{r_3^\alpha}{r_1^{\alpha+1}}\quad\text{according as } r_1\leqslant r_3 \text{ or } r_1\geqslant r_3 \quad (7.4)$$

II. Integration of Angular Part

§ 8. $2p^2$-*configuration.* For O_{III}-ion, $2p^2$-configuration forms a group of lowest levels; levels of other configurations lying far above it. Hence from the astrophysical point of view, we may limit ourselves to consider the transitions occuring within the levels[1] of this configuration. The energy levels of this configuration are ${}^1S_0$, ${}^1D_2$ and ${}^3P$ (cf. fig. 1 of our previous paper), and can be characterized fairly approximately by the Russell-Saunder coupling. In analogy to the terminology of J. C. Boyce and others[2] with respect to the forbidden transitions, we use the words *nebular excitation* for the impact excitation ${}^3P\to{}^1D_2$, *auroral excitation* for ${}^1D_2\to{}^1S_0$, and *transauroral excitation* for ${}^3P\to{}^1S_0$.

§ 9. To integrate $f_{mn'}(\theta)$ and $g_{mn'}(\theta)$, we must first express the eigen-functions of the state in terms of the zero-order states $u(n, l, m_l, m_s)$, characterized by the set of quantum numbers n, l, m_l, m_s of individual electrons:

$$\Psi({}^3P_0^0)=\frac{1}{\sqrt{3}}\Big[\Phi(0^+,-1^+)-\frac{1}{\sqrt{2}}$$
$$\times\{\Phi(1^+,-1^-)+\Phi(1^-,-1^+)\}+\Phi(1^-,0^-)\Big]$$

1. Following E. U. Condon, we use throughout this paper the word *state* as a quantum state without any degeneration and *level* as an ensemble of states which have approximately the same energy. Cf. Condon and Shortley, The Theory of Atomic Spectra (1934) 217.

2. J. C. Boyce, D. H. Menzel and C. H. Payne, Proc. Nat. Acad. Sci. **19** (1933) 581,

$$\Psi(^3P_1^1)=\frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}\{\Phi(1^+,0^-)+\Phi(1^-,0^+)\}-\Phi(1^+,-1^+)\right]$$
$$\Psi(^3P_1^0)=\frac{1}{\sqrt{2}}[\Phi(1^-,0^-)-\Phi(0^+,-1^+)]$$
$$\Psi(^3P_1^{-1})=\frac{1}{\sqrt{2}}\left[\Phi(1^-,-1^-)-\frac{1}{\sqrt{2}}\{\Phi(0^+,-1^-)+\Phi(0^-,-1^+)\}\right]$$
$$\Psi(^3P_2^2)=\Phi(1^+,0^+)$$
$$\Psi(^3P_2^1)=\frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}\{\Phi(1^+,0^-)+\Phi(1^-,0^+)\}+\Phi(1^+,-1^+)\right]$$
$$\Psi(^3P_2^0)=\frac{1}{\sqrt{6}}[\Phi(1^-,0^-)+\sqrt{2}\{\Phi(1^+,-1^-)+\Phi(1^-,-1^+)\}$$
$$+\Phi(0^+,-1^+)]$$
$$\Psi(^3P_2^{-1})=\frac{1}{\sqrt{2}}\left[\Phi(1^-,-1^-)+\frac{1}{\sqrt{2}}\{\Phi(0^+,-1^-)+\Phi(0^-,-1^+)\}\right]$$
$$\Psi(^3P_2^{-2})=\Phi(0^-,-1^-)$$
$$\Psi(^1D_2^2)=\Phi(1^+,1^-)$$
$$\Psi(^1D_2^1)=\frac{1}{\sqrt{2}}[\Phi(1^+,0^-)-\Phi(1^-,0^+)]$$
$$\Psi(^1D_2^0)=\frac{1}{\sqrt{6}}[\Phi(1^+,-1^-)-\Phi(1^-,-1^+)+2\Phi(0^+,0^-)]$$
$$\Psi(^1D_2^{-1})=\frac{1}{\sqrt{2}}[\Phi(0^+,-1^-)-\Phi(0^-,-1^+)]$$
$$\Psi(^1D_2^{-2})=\Phi(-1^+,-1^-)$$
$$\Psi(^1S_0^0)=\frac{1}{\sqrt{3}}[\Phi(1^+,-1^-)-\Phi(1^-,-1^+)-\Phi(0^+,0^-)] \qquad (9.1)$$

where we denote the wave functions as $\Psi(^{2S+1}L_J^M)$ instead of $\Psi_n(\boldsymbol{n}_1, \boldsymbol{n}_2)$, and for any two electrons a and b we put

$$\Phi(m_l^\pm, m_l'^\pm)=\frac{1}{\sqrt{2}}\begin{vmatrix}\omega_a(m_l^\pm) & \omega_b(m_l^\pm)\\ \omega^a(m_l'^\pm) & \omega_b(m_l'^\pm)\end{vmatrix}, \qquad (9.2)$$

where spin components are specified by superscribing signs $\pm$; and $\omega(m_l^\pm)$ means the angular part of the wave function $u(n, l, m_l. m_s)$, viz.

$$u(n, l, m_l, m_s)=\frac{R_{nl}(r)}{r}\omega(m_l^\pm), \qquad (9.3)$$

where

$$\omega(m_l^\pm)=\Theta(l, m_l)\Phi(m_l)\sigma(m_s) \qquad (9.4)$$

$$\Theta(l, m)=(-)^m\sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)$$
$$\Theta(l, -m)=\sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta) \quad (m\geqq 0) \qquad (9.5)$$

$$\Phi(m)=\frac{1}{\sqrt{2\pi}}e^{im\phi} \tag{9.6}$$

and $\sigma(m_s)$, the spin eigen-function. We shall use afterwards the notation $\omega(m_l)$ dropping the spin factor from $\omega(m_l^{\pm})$, i. e.

$$\omega(m_l)=\Theta(l, m_l)\Phi(m_l) \tag{9.7}$$

§ 10. *Exchange term.* Integrating (7.2) with respect to v_2 and spin coordinates of 1-and 3-electrons, we obtain

$$g_{nn'}(\theta)=\frac{-1}{2\pi a_0}\int_0^\infty R(r_1)R(r_3)r_1r_3dr_1dr_3Z(n, n'), \tag{10.1}$$

where Z is given in Table I.

Table I.

transition	Z	transition	Z
I. ${}^1D_2\to{}^1S_0$		${}^3P_1^{\pm1}$, ${}^1D_2^{\pm1}$	$\frac{1}{4}\zeta_{10}$
${}^1D_2^{\pm2}$, ${}^1S_0^0$	$\frac{1}{\sqrt{3}}\zeta_{11}$	${}^3P_1^0$, ${}^1D_2^{\pm1}$	$\frac{1}{4}(\zeta_{00}-\zeta_{-11}+\zeta_{11})$
${}^1D_2^{\pm1}$, ${}^1S_0^0$	$\frac{1}{\sqrt{6}}(\zeta_{10}-\zeta_{01})$	${}^3P_1^{\pm1}$, ${}^1D_2^0$	0
${}^1D_2^0$, ${}^1S_0^0$	$-\sqrt{\frac{2}{3}}(\zeta_{00}+\zeta_{-11})$	${}^3P_1^0$, ${}^1D_2^0$	0
II. ${}^3P\to{}^1S_0$		${}^3P_2^2$, ${}^1D_2^2$	$\frac{1}{2}\zeta_{01}$
${}^3P_0^0$, ${}^1S_0^0$	$\frac{1}{3}(\zeta_{10}+\zeta_{01})$	${}^3P_2^{-2}$, ${}^1D_2^{-2}$	$\frac{1}{2}\zeta_{01}$
${}^3P_1^{\pm1}$, ${}^1S_0^0$	0	${}^3P_2^2$, ${}^1D_2^{-2}$	0
${}^3P_1^0$, ${}^1S_0^0$	0	${}^3P_2^{-2}$, ${}^1D_2^2$	0
${}^3P_2^{\pm2}$, ${}^1S_0^0$	$\frac{1}{2\sqrt{3}}(\zeta_{10}+\zeta_{01})$	${}^3P_2^{\pm1}$, ${}^1D_2^{\pm2}$	$\frac{1}{2\sqrt{2}}\zeta_{11}$
${}^3P_2^{\pm1}$, ${}^1S_0^0$	0	${}^3P_2^0$, ${}^1D_2^{\pm2}$	$\frac{1}{2\sqrt{6}}\zeta_{01}$
${}^3P_2^0$, ${}^1S_0^0$	$\frac{1}{3\sqrt{2}}(\zeta_{10}+\zeta_{01})$	${}^3P_2^2$, ${}^1D_2^1$	$\frac{1}{2\sqrt{2}}(\zeta_{-11}-\zeta_{00})$
III. ${}^3P\to{}^1D_2$		${}^3P_2^{-2}$, ${}^1D_2^{-1}$	$\frac{1}{2\sqrt{2}}(\zeta_{-11}-\zeta_{00})$
${}^3P_0^0$, ${}^1D_2^{\pm2}$	$\frac{1}{2\sqrt{3}}\zeta_{01}$	${}^3P_2^2$, ${}^1D_2^{-1}$	$\frac{1}{2\sqrt{2}}\zeta_{11}$
${}^3P_0^0$, ${}^1D_2^{\pm1}$	$\frac{1}{2\sqrt{6}}(\zeta_{00}-\zeta_{-11}-\zeta_{11})$	${}^3P_2^{-2}$, ${}^1D_2^1$	$\frac{1}{2\sqrt{2}}\zeta_{11}$
${}^3P_0^0$, ${}^1D_2^0$	$\frac{\sqrt{2}}{6}\zeta_{01}-\sqrt{\frac{2}{3}}\zeta_{10}$	${}^3P_2^{\pm1}$, ${}^1D_2^{\pm1}$	$\frac{1}{4}\zeta_{10}$
${}^3P_1^{\pm1}$, ${}^1D_2^{\pm2}$	$\frac{1}{2\sqrt{2}}\zeta_{11}$	${}^3P_2^0$, ${}^1D_2^{\pm1}$	$\frac{1}{4\sqrt{3}}(\zeta_{00}-\zeta_{11}-\zeta_{-11})$
${}^3P_1^0$, ${}^1D_2^{\pm2}$	$\frac{1}{2\sqrt{2}}\zeta_{01}$	${}^3P_2^{\pm2}$, ${}^1D_2^0$	$\frac{1}{2\sqrt{6}}(2\zeta_{10}-\zeta_{01})$
		${}^3P_2^{\pm1}$, ${}^1D_2^0$	0
		${}^3P_2^0$, ${}^1D_2^0$	$\frac{1}{6}(2\zeta_{10}-\zeta_{01})$

$\zeta_{m_l m_l'}$ is the quantity obtained from the angular part of $g_{nn'}(\theta)$ on replacing $\Psi_{n'}^{*}\Psi_{n}$ by $\omega_1(m_l)\omega_3(m_l')$:

$$\zeta_{m_l m_l'}=\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}\int\omega_1(m_l)\omega_3(m_l')\gamma_\alpha\frac{(\alpha-|\beta|)!}{(\alpha+|\beta|)!}P_\alpha^{|\beta|}(\cos\theta_1)P_\alpha^{|\beta|}(\cos\theta_3)$$
$$\times e^{i(\phi_1-\phi_3)}e^{i(k\boldsymbol{n}_0\boldsymbol{r}_3-k'\boldsymbol{n}\boldsymbol{r}_1)}\sin\theta_1\sin\theta_3 d\theta_1 d\theta_3 d\phi_1 d\phi_3. \tag{10.2}$$

For transauroral and nebular excitations, viz. for cases II and III in Table I, sign of $Z(n, n')$ is omitted, since $f_{nn'}(\theta)$ vanishes in these cases, and the sign of $g_{nn'}(\theta)$ becomes indifferent to the calculation of the scattering intensity. (cf. § 17).

§ 11. We have next to evaluate $\zeta_{m_l m_l'}$. The result of calculation is as follows:

$$\zeta_{11}=\zeta_{-1-1}=3\pi^2(kr_3)^{-3/2}(k'r_1)^{-1/2}\sum_{\alpha=1}^{\infty}\frac{1}{2\alpha+1}$$
$$\times\gamma_\alpha J_{\alpha+1/2}(kr_3)[P_{\alpha+1}^2(\cos\theta)J_{\alpha+3/2}(k'r_1)+P_{\alpha-1}^2(\cos\theta)J_{\alpha-1/2}(k'r_1)]$$
$$\zeta_{1-1}=\zeta_{-11}=-3\pi^2(kr_3)^{-3/2}(k'r_1)^{-1/2}\sum_{\alpha=1}^{\infty}\frac{\alpha(\alpha+1)}{2\alpha+1}$$
$$\times\gamma_\alpha J_{\alpha+1/2}(kr_3)[P_{\alpha+1}(\cos\theta)J_{\alpha+3/2}(k'r_1)+P_{\alpha-1}(\cos\theta)J_{\alpha-1/2}(k'r_1)]$$
$$\zeta_{01}=\zeta_{0-1}=-3\pi^2(kr_3)^{-3/2}(k'r_1)^{-1/2}\sum_{\alpha=1}^{\infty}\frac{1}{2\alpha+1}\gamma_\alpha J_{\alpha+1/2}(kr_3)$$
$$\times[\alpha P_{\alpha+1}^1(\cos\theta)J_{\alpha+3/2}(k'r_1)+(\alpha+1)P_{\alpha-1}^1(\cos\theta)J_{\alpha-1/2}(k'r_1)]$$
$$\zeta_{10}=\zeta_{-10}=-i3\pi^2(kr_3)^{-1/2}(k'r_1)^{-1/2}\sum_{\alpha=0}^{\infty}\frac{1}{(2\alpha+1)^2}\gamma_\alpha[(\alpha+1)J_{\alpha+3/2}(kr_3)$$
$$-\alpha J_{\alpha-1/2}(kr_3)][P_{\alpha+1}^1(\cos\theta)J_{\alpha+3/2}(k'r_1)+P_{\alpha-1}^1(\cos\theta)J_{\alpha-1/2}(k'r_1)]$$
$$\zeta_{00}=3\pi^2(kr_3)^{-1/2}(k'r_1)^{-1/2}\sum_{\alpha=0}^{\infty}\frac{1}{(2\alpha+1)^2}\gamma_\alpha[(\alpha+1)J_{\alpha+3/2}(kr_3)-\alpha J_{\alpha+1/2}(kr_3)]$$
$$\times[(\alpha+1)P_{\alpha+1}(\cos\theta)J_{\alpha+3/2}(k'r_1)-\alpha P_{\alpha-1}(\cos\theta)J_{\alpha-1/2}(k'r_1)], \tag{11.1}$$

where P and J are Legendre and Bessel functions respectively.

§ 12. *Direct term.* $f_{nn'}(\theta)$ vanishes for intersystem excitations, since the initial and the final levels are of opposite symmetry. Thus this term appears only in the auroral excitation, ${}^1D_2\rightarrow{}^1S_0$.

The computation of $f_{nn'}(\theta)$ of (6.5) is similar to the previous case. The angular part of $f_{nn'}(\theta)$ is expressed by the linear combination of terms such as

$$\eta_{m_l, m_l';\, m_l'', m_l'''}=\int(\sum_\alpha e^{i(k\boldsymbol{n}_0-k'\boldsymbol{n})\boldsymbol{r}_\alpha})$$
$$\times\omega_1(m_l)\omega_1(m_l')\omega_2(m_l'')\omega_2(m_l''')\sin\theta_1\sin\theta_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2. \tag{12.1}$$

η vanishes if both m_l+m_l' and $m_l''+m_l'''$ differ from zero.
Integrating it, we obtain finally,

$$f_{nn'}(\theta)=\frac{-1}{2a_0K'^2}\int_0^\infty R^2(r)X(n, n')dr \tag{12.2}$$

$$X({}^1D_2^{\pm2}, {}^1S_0^0) = \frac{2}{\sqrt{3}} \eta_{1,1;1,-1}$$

$$X({}^1D_2^{\pm1}, {}^1S_0^0) = \sqrt{\frac{2}{3}} (\eta_{1,-1;1,0} - \eta_{0,0;0,1}) \qquad (12.3)$$

$$X({}^1D_2^0, {}^1S_0^0) = \frac{\sqrt{2}}{3} (\eta_{1,-1;1,-1} - \eta_{0,0;0,1})$$

$$\eta_{1,1;1,-1} = \eta_{-1,-1;1,-1} = -\frac{3}{4}\sqrt{\frac{2\pi}{rK'}} \sin^2\psi J_{5/2}(rK')$$

$$\eta_{1,-1;1,0} = \eta_{1,-1;-1,0} = \frac{3}{4}\sqrt{\frac{2\pi}{rK'}} \sin\psi J_{3/2}(rK')$$

$$\eta_{0,0;0,1} = \eta_{0,0;0,-1} = \frac{-3i}{8}\sqrt{\frac{2\pi}{rK'}}$$

$$\cos\psi \sin\psi J_{5/2}(rK') \qquad (12.4)$$

$$\eta_{1,-1;1,-1} = \sqrt{\frac{2\pi}{rK'}} (J_{1/2}(rK') + P_2(\cos\psi) J_{5/2}(rK'))$$

$$\eta_{0,0;0,0} = \frac{1}{4}\sqrt{\frac{2\pi}{rK'}} (J_{1/2}(rK') - 2P_2(\cos\psi) J_{5/2}(rK'))$$

$$\sin\psi = k' \sin\theta / K' \qquad (12.5)$$

III. Integration of Radial Part.

§ 13. *Exchange term.* As is seen from (10.1) and Table I, $g_{mm'}(\theta)$ is given by the linear combination of terms such as

$$g_{[m_l, m_l']}(\theta) = \frac{-1}{2\pi a_0} \int R(r_1) R(r_3) \zeta_{m_l, m_l'} r_1 r_3 dr_1 dr_3. \qquad (13.1)$$

To work out this integral, we first transform r and k to the atomic scale by putting:

$$\xi = r/a_0, \qquad \varkappa = k a_0 \qquad \text{and } \varkappa' = k' a_0 \qquad (13.2)$$

If we designate by $\zeta_{m_l, m_l'}(\xi, \varkappa)$ the expression which is obtained formally from $\zeta_{m_l m_l'}$ by replacing r and k therein by the new variables ξ and $\varkappa$, we get

$$g_{[m_l, m_l']}(\theta) = \frac{-a_0}{2\pi} \int R(\xi_1) R(\xi_3) \zeta_{m_l, m_l'}(\xi, \varkappa) \xi_1 \xi_3 d\xi_1 d\xi_3. \qquad (13.3)$$

For 2p-electron, the radial part $R(\xi)$ is well represented by the simple exponential function,

$$R(\xi) = \xi^2 (a e^{-c\xi} + b e^{-d\xi}) = \xi^2 \bar{R}(\xi), \qquad (13.4)$$

where a, b and c, d are characteristic constants of the ion.

From (13.3), (13.4) and (11.1) we obtain after some calculation,

$$g_{[1,1]}(\theta) = \frac{-3\pi}{2} a_0 \sum_{\alpha=1}^{\infty} \frac{1}{2\alpha+1} \int_0^\infty \bar{R}(\xi_3) \frac{\xi_3^3}{(\varkappa\xi_3)^{3/2}} J_{\alpha+1/2}(\varkappa\xi_2)$$

$$\times\left[\xi_3^{\alpha}\left\{P_{\alpha+1}^2(\theta)\int_{\xi_3}^{\infty}\bar{R}(\xi_1)\frac{J_{\alpha+3/2}(\varkappa'\xi_1)}{\sqrt{\varkappa'\xi_1}}\xi_1^{2-\alpha}d\xi_1+P_{\alpha-1}^2(\theta)\right.\right.$$
$$\left.\times\int_{\xi_3}^{\infty}\bar{R}(\xi_1)\frac{J_{\alpha-1/2}(\varkappa'\xi_1)}{\sqrt{\varkappa'\xi_1}}\xi_1^{2-\alpha}d\xi_1\right\}+\frac{1}{\xi_3^{\alpha+1}}\left\{P_{\alpha+1}^2(\theta)\int_0^{\xi_3}\bar{R}(\xi_1)\frac{J_{\alpha+3/2}(\varkappa'\xi_1)}{\sqrt{\varkappa'\xi_1}}\right.$$
$$\left.\left.\times\xi_1^{\alpha+3}d\xi_1+P_{\alpha-1}^2(\theta)\int_0^{\xi_3}\bar{R}(\xi_1)\frac{J_{\alpha-1/2}(\varkappa'\xi_1)}{\sqrt{\varkappa'\xi_1}}\xi_1^{\alpha+3}d\xi_1\right\}\right]d\xi_3 \qquad (13.5)$$

and similar expressions.

$\varkappa'\xi$ is small for the case of astrophysical interest. Hence, this can be evaluated by the series expansion. Formulae are too complicated to reproduce here.

§ 14. *Direct term.* $f_{mm'}(\theta)$ is also given by the linear combination of

$$f[m_l, m_l' : m_l'', m_l'''](\theta)=\frac{-1}{2a_0K'^2}\int_0^{\infty}R^2(r)\eta_{m_l, m_l' ; m_l'', m_l'''}dr. \qquad (14.1)$$

Making the transformation (13.2), we have

$$f[m_l, m_l' ; m_l'', m_l'''](\theta)=\frac{-a_0}{2K^2}\int_0^{\infty}R^2(r)\eta_{m_l, m_l ; m_l'', m_l'''}(\xi, \varkappa)d\xi, \quad (14.2)$$

where

$$K^2=\frac{1}{a_0}K'^2=\varkappa^2+\varkappa'^2-2\varkappa\varkappa'\cos\theta. \qquad (14.3)$$

$\eta_{m_l, m_l' ; m_l'', m_l'''}(\xi, \varkappa)$ is the expression which is obtained from $\eta_{m_l, m_l' ; m_l'', m_l'''}$ by replacing formally ξ and K, for r and K' respectively, although η does not alter its value by such substitution in the present case.

Evaluation of (14.2) is simple. We obtain

$$f_{[1,1;1,-1]}(\theta)=\sqrt{\pi}\,a_0\frac{1}{(2K)^{5/2}}P_2^2(\cos\psi)\Omega\binom{5/2+1}{5/2}$$

$$f_{[1,-1;1,0]}(\theta)=\sqrt{\pi}\,a_0\frac{-1}{(2K)^{5/2}}P_1^1(\cos\psi)\Omega\binom{3/2+2}{3/2}$$

$$f_{[0,0;0,1]}(\theta)=\sqrt{\pi}\,a_0\frac{i}{2(2K)^{5/2}}P_2^1(\cos\psi)\Omega\binom{5/2+1}{5/2}$$

$$f_{[1,-1;1,-1]}(\theta)=\sqrt{\pi}\,a_0\frac{-4}{(2K)^{5/2}}\left[\Omega\binom{1/2+3}{1/2}+P_2(\cos\psi)\Omega\binom{5/2+1}{5/2}\right]$$

$$f_{[0,0;0,0]}(\theta)=\sqrt{\pi}\,a_0\frac{-1}{(2K)^{5/2}}\left[\Omega\binom{1/2+3}{1/2}-2P_2(\cos\psi)\Omega\binom{5/2+1}{5/2}\right]. \quad (14.4)$$

where $$\Omega\binom{x}{y}=a^2I_y^x(2c, K)+2abI_y^x(c+d, K)+b^2I_y^x(2d, K) \quad (14.5)$$

$$I_y^x(c, K)=\int_0^{\infty}e^{-c\xi}J_y(K\xi)\xi^x d\xi.$$

IV. Effective Cross Section

§ 15. *Hartree Field for O_{III}.* It is well know that a complex atom is well characterized by the Hartree fields, which is given in a style of numerical table. But it is incovenient for practical use. J. C. Slater[1] has pointed out that they can be reproduced with considerable order of accuracy by some simple analytic expressions. In our calculation, Hartree field for 2p-state appears in the expression of $g_{mm'}(\theta)$ and $f_{mm'}(\theta)$, as the factor $R(\xi)$. Hartree Field for O_{III} has been already obtained by himself and M. M. Black[2], so that we are only to determine the constants in the analytic expression (13.4). Following T. R. Running's method[3] we obtain

$$a=5.00 \qquad b=11.5 \qquad c=2.03 \qquad d=3.98 \qquad (15.1)$$

§ 16. *Energy of $2p^2$-configuration.* There are three levels ^3P, $^1D_2$, and $^1S_0$ in $2p^2$-configuration. Since they are all of the same symmetry, transitions within them are not dipole. E. U. Condon[4] shows that even magnetic dipole and quadrupole transition probability vanish for $^1D_2 \rightarrow {}^2P_0$ and $^1S_0 \rightarrow {}^3P_0$ and this is nearly so for $^1S_0 \rightarrow {}^3P_2$. Of remaining four transitions, three which are associated with the emission lines in observable region, are of astrophysical interest. They are observed in gaseous nebulae: nebular lines $N_1(^1D_2 \rightarrow {}^3P_1)$, $N_2(^1D_2 \rightarrow {}^3P_2)$ of wave length λ 5007 Å and λ 4959 Å respectively, and auroral line $^1S_0 \rightarrow {}^1D_2$ at λ 4363 Å.

The energy differences within these levels, expressed in terms of equivalent electron velocity, v, are as follows.

Table II.

	$^3P_1-{}^1D_2$	$^3P_2-{}^1D_2$	$^1D_2-{}^1S_0$	$^3P_1-{}^1S_0$	$^3P_2-{}^1S_0$
v in 10^8 cm/sec	0.936	0,932	0.998	1.368	1.365

These v are just the threshold value for each excitation. For instance, the colliding electron must have the velocity larger than 0.936×10^8 cm/sec to excite the ion from $^3P_1$ to $^1D_2$.

§ 17. *Effective cross section.* As has been stated in § 4, we assume that the elctrons of saturated shells are concerned only with

1. L. C. Slater, Phys. Rev. **42** (1932) 33.
2. D. R. Hartree and M. M. Black, Proc. Roy. Soc. A. **139** (1933) 311.
3. T. R. Running, Empirical Formulas (1917) § 17.
4. E. U. Condon, Ap. J. **79** (1934) 217.

the average atomic field, and that the 2p-and the impinging electons obey Fermi statistics. Then, for the unpolarized beam of the impinging electron, both $f_{nn'}(\theta)$ and $g_{nn'}(\theta)$ are to be combined with to give the scattering intensity as

$$I_{nn'}(\theta)d\omega=\frac{k'}{k}|f_{nn'}(\theta)-g_{nn'}(\theta)|^2d\omega, \tag{17.1}$$

where $d\omega$ means elementary solid angle.

The effective cross section of the excitedation $n\rightarrow n'$ is then given by

$$Q_{nn'}(v)=2\pi\int_0^\infty I_{nn'}(\theta)\sin\theta d\theta. \tag{17.2}$$

$Q_{nn'}$ between *states* n and n' are combined to give the cross section between *levels* ${}^1S_0^0, {}^1D_2$ and ${}^3P$ as follows:

Auroral dxcitation $\quad Q_{DS}(v)=\frac{1}{5}\sum_M Q_{{}^1D_2^M\rightarrow{}^1S_0^0}(v)$

Transauroral excitation $\quad Q_{PS}(v)=\frac{1}{9}\sum_{J,M} Q_{{}^3P_J^M\rightarrow{}^1S_0^0}(v)$

Nebular excitation $\quad Q_{PD}(v)=\frac{1}{9}\sum_{J,M,M'} Q_{{}^3P_J^M\rightarrow{}^1D_2^{M'}}(v).$

Summation must be extended to all possible values of M; J, M; J, M, M'. There, 5 and 9 are the statistical weight of level ${}^1D_2$ and ${}^3P$ respectively.

§ 18. Preliminary results of the numerical computation are given in Table III. We have restricted onr computation within the velocity range $v\leqq3\times10^8$ cm/sec, which is sufficient for astrophysical application.

Table III. $Q(v)$ for O_{III} in unit of πa_0^2.

Transition	$v.10^{-8}$	1.0	1.25	1.5	1.75	2.0	2.5	3.0
Aur.	${}^1D_2\rightarrow{}^1S_0^0$	0.086	4.2	6.4	7.2	6.7	6.7	(8.2)
Tr. Aur.	${}^3P\rightarrow{}^1S_0^0$			0.0026	0.014	0.027	0.072	(0.089)
Neb.	${}^3P\rightarrow{}^1D_2$	0.14	0.18	0.23	0.28	0.32	0.54	(0.92)

For $v\leqq2\times10^8$ cm/sec, the exchange term is easily computed by the series expansion. With increasing v, convergence of the series becomes worse. In the present calculation, v for 3×10^8 is much uncertain.

Though we have not extended our calculation to larger v, it seems that for most of $Q(v)$ their maxima lie between $v=(3\pm1\times10^8$.

It is also clear from the general consideration that $Q(v)$ decreases rapidly for larger v. And especially so for nebular and transauroral cases, where $f(\theta)$-term vanishes leaving $g(\theta)$.

Large cross section for auroral excitation comes from its $f(\theta)$-terms which is very large for small θ. In other words, the dominant process in this case is the direct excitation resulting in the small deflection. On the contrary, exchange excitation shows a much more uniform distribution of the scattering electron,

To evaluate the cross sections among states of the level ^3P, more accurate treatment than ours is necessary.

As has been noted in § 4, theoretical cross section seems to be much affected by the starting assumption. Exact solution will give larger cross section than our plane wave approximation. More accurate treatment is desirable.

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