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Erratum

Equation (3.15e) should be further reduced to

$$\sigma_q(22) = \sum_{MM'} (-)^{M-M'} \langle FFM(q-M)\,|2q\rangle \langle FFM'(q-M')\,|2q\rangle$$

$$\times\ 2\pi \int [\delta_{MM'} - \langle \alpha FM|S_c|\alpha FM'\rangle \langle \alpha F(M-q)\,|S_c|\,\alpha F(M'-q)\rangle^*]\ b\ db. \qquad (3.15e)$$

Atomic States and Collisional Relaxation in Plasma Polarization Spectroscopy: Axially Symmetric Case

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Prefatory Note

Several years ago we started our attempts to develop Plasma Polarization Spectroscopy (PPS), under the auspices of the then Institute of Plasma Physics, and later of the Natinal Institute for Fusion Science. In the early stage of our activities, we put some emphasis on establishing a perspective of our present knowlege on the elements of PPS, *i.e.*, individual atomic processes. We collected the atomic data pertinent to PPS, and the first batch of the outcome appeared as a report in this series, "*Atomic Processes Relevant to Polarization Plasma Spectroscopy*" (NIFS-DATA-16, 1992). Fortunately, this received much interest, and copies of the report have all run out.

Originating from the above activities, the circle of PPS expanded to the U.S., first to Los Alamos National Laboratory and then to Jet Propulsion Laboratory. In February 1994, The First Japan-U.S. Workshop on Plasma Polarization Spectroscopy was held at Los Alamos National Laboratory. This meeting was attended by all the major researchers in this area, including the pioneers from Russia, Canada and France. Now the efforts in this new field is being united internationally.

In the course of the above developments, we began to construct a basic framework for PPS. It was our common understanding that our sound footing should be the collisional-radiative model which has been well established as the most comprehensive method to treat the populations of excited atoms and ions in a plasma. We decided to expand this method so that our new method can treat alignment of excited atoms and ions as well; this quantity is responsible for the polarization of an emission line. This attempt turned out not to be an easy task and it took an unduly long time to complete the manuscript. This report is thus the second batch of our efforts. We hope this report, like the former one, receives many interested readers.

In this volume, the basic formalism is established for the ionizing plasma component. In view of the recent experimental observations, we feel we have to expand the present formalism so as to include the recombining plasma component as well. We hope we can accomplish that in the near future.

Finally, we would like to express our gratitude to the National Institute for Fusion Science for its continued support of our endeavor.

August, 1996

Abstract

An ensemble of atoms (or ions) is described in terms of the density matrix, and two quantities, *population* and *alignment*, are assigned to each atomic level for axially symmetric plasma environment. Collisional relaxation is treated semiclassically as transitions between vectors in the Liouville space and interpreted as elastic or inelastic transitions among the population and the alignment of the levels. A spatially anisotropic velocity distribution of perturbers is expanded in terms of Legendre polynomials, and rate coefficients are defined for the transitions. A set of rate equations are constructed for the system of populations and another set for that of alignments. In the case of an isotropic Maxwellian distribution of perturbers the former reduces to the conventional collisional-radiative model describing the ionizing plasma component of populations. As an example, berylliumlike oxygen in an anisotropic plasma environment is treated by this method.

keywords: population, alignment, anisotropy, velocity distribution, density matrix, collisional relaxation, polarization, collisional-radiative model

1 Introduction

In conventional plasma spectroscopy little attention was paid in the past to polarization phenomena. In recent years, however, in various important devices and experimental situations plasmas have been created that are spatially anisotropic, which in turn would result in the emission of polarized radiation. Examples of such devices and experiments are: the creation of suprathermal electrons in tokamaks, neutral beam injection for heating and for diagnostics of magnetic fusion energy (MFE) devices, the creation of electrons with anisotropic velocity distribution in laser-produced plasmas, and similar phenomena in laser-induced fluorescence spectroscopy. Under the above conditions excited atoms or ions (to which we shall refer in the future as *atoms*) are produced by atomic collision processes that are spatially anisotropic making these atoms polarized. In many cases alignment is produced. Radiation emitted by these atoms will be linearly polarized and will have a spatially anisotropic intensity distribution. Plasma Polarization Spectroscopy (PPS) is the new field of research in which the polarization characteristics of the radiation emitted by the plasma is used for the purposes of obtaining information about the plasma, especially about its spatial anisotropy and therefore its non-thermal characteristics (Kazantsev and Hénoux, 1995).

This report is a step to establish the theoretical framework of PPS. We develop a formalism within the semiclassical approximation, pertinent mainly to heavy-particle collisions but also applicable as an approximation for electronic collisions.

First, we shall introduce the density-matrix description of an atomic ensemble (§2). In §3 we shall introduce the master equation for the density matrix that contains the relaxation matrix, and we shall discuss the calculation of the relaxation matrix for monoenergetic perturbers in the semi-classical approximation. In §4 we shall extend the formulas to a realistic velocity distribution of perturbers and obtain rate equations for population and for alignment. Finally, in §5 we shall give an example. Our presentation is based on that of Omont (1977).

2 Density-matrix description of atomic ensembles

Let $|\alpha FM\rangle$ be the standard representation for the atomic states, where F

and M label the total angular momentum and its projection onto the z-axis, respectively, and α denotes the other indices necessary to specify the state. The atomic density matrix then can be written in the form,

$$\rho = \sum_{\alpha FM\beta GN} \rho_{\alpha FM,\, \beta GN} \,|\, \alpha FM\rangle \langle \beta GN|. \tag{2.1}$$

In place of $|\,\alpha FM\rangle\langle\beta GN|$, we introduce the irreducible sets

$$T^{(k)}{}_q(\alpha F, \beta G) = \sum_N (-)^{G-N} \langle FGM-N|kq\rangle \,|\, \alpha FM\rangle \langle \beta GN|, \tag{2.2}$$

where $\langle FGM-N|kq\rangle$ is the Clebsch–Gordan coefficient. These $T^{(k)}{}_q$'s may be considered as vectors of the Liouville space, of which they form a standard irreducible basis. The density matrix can be expanded with respect to this basis as,

$$\rho = \sum_{\alpha\beta FG,\, kq} \rho^k{}_q(\alpha F, \beta G)\; T^{(k)}{}_q(\alpha F, \beta G). \tag{2.3}$$

By using the relationship

$$\mathrm{Tr}\{T^{(k)}{}_q(\alpha F, \beta G)\, T^{(k')}{}_{q'}(\alpha' F', \beta' G')^\dagger\} = \delta_{\alpha\alpha'}\, \delta_{FF'}\, \delta_{\beta\beta'}\, \delta_{GG'}\, \delta_{kk'}\, \delta_{qq'} \tag{2.4}$$

we can express the irreducible components $\rho^k{}_q(\alpha F, \beta G)$ as

$$\rho^k{}_q(\alpha F, \beta G) = \sum_N (-)^{G-N} \langle FGM-N|kq\rangle\, \rho_{\alpha FM,\, \beta GN}. \tag{2.5}$$

In the later part of this article, we will consider situations where the following *three assumptions* hold;

i) Axial symmetry is present around the z-axis, the quantization axis.

ii) There is no coherence among the different Zeeman multiplets (optical coherence or Hertzian coherence) and among the different magnetic sublevels in a Zeeman multiplet (Zeeman coherence). These assumptions imply that $\rho_{\alpha FM,\, \beta GN} = 0$ for $\alpha \neq \beta$ and $\rho_{\alpha FM,\, \alpha FM'} = 0$ for $M \neq M'$. In effect our assumptions imply that the state considered is an incoherent superposition of atomic 'level states' and each atomic 'level state' is an incoherent superposition of its Zeeman sublevel states. We put $\beta G = \alpha F$ and denote this level simply as p or r.

iii) Electric and magnetic fields are absent.

Under these conditions, the density matrix, given by eq. (2.3), reduces to a sum of density matrices for each Zeeman multiplet, say level p, as

$$\rho(p) = \rho^0{}_0(p)T^{(0)}{}_0(p) + \rho^2{}_0(p)T^{(2)}{}_0(p) + \cdots . \qquad (2.6)$$

3 The relaxation matrix in the semi-classical approximation

The time development of the system due to a relaxation mechanism may be described in terms of the relaxation matrix G

$$(\mathrm{d}\rho/\mathrm{d}t)_{relax} = -G\rho. \qquad (3.1)$$

In the dyadic representation this equation can be written as,

$$(\mathrm{d}\rho_{ij}/\mathrm{d}t)_{relax} = -\sum_{rs} G_{ij,\,rs}\,\rho_{rs}, \qquad (3.2)$$

with

$$G_{ij,\,rs} = \langle\langle ij^{+}|G|rs^{+}\rangle\rangle, \qquad (3.3)$$

where $|\ ^{+}\rangle\rangle$ denotes a vector in the Liouville space. It can be easily seen (and understood physically) that if initially an atomic state was described by $\rho(p)$ as given by eq. (2.6), it will remain so at all times; *i.e.*, eq. (2.6) can be assumed to be correct at later times also.

We now consider the effect of collisions in the *semi-classical approximation*. We assume a rectilinear path. A collision is defined by the relative velocity $\boldsymbol{v}$ and the impact parameter $\boldsymbol{b}$ ($\boldsymbol{b}\cdot\boldsymbol{v} = 0$). The time development of the density matrix is described in terms of the S matrix, which is equal to the time evolusion operator $U(\infty,-\infty)$, and is given by

$$(\mathrm{d}\rho/\mathrm{d}t)_{coll} = -G_c\rho = 2\pi n_p\langle v\int b\,\mathrm{d}b\,[S(b,v)\,\rho\,S(b,v)^{\dagger} - \rho]\rangle_{Av}, \qquad (3.4)$$

where n_p is the density of perturbers and the average is over the velocities and the directions of $\boldsymbol{b}$.

3.1 Monoenergetic beam perturbers and cross sections

We first consider monoenergetic beam perturbers with velocity $\boldsymbol{v}$ in the z'-direction. We define an intermediate "superoperator" matrix $\tilde{\Pi}(b, v)$ by averaging over the directions of $\boldsymbol{b}$ (perpendicular to $\boldsymbol{v}$).

$$\tilde{\Pi}(b, v)\,\rho = \rho - \{S_c\,\rho\,S_c{}^{\dagger}\}_{bAv}, \tag{3.5}$$

where the index c means that the matrix S is referred to these collision axes. The matrix elements of $\tilde{\Pi}$ are

$$\begin{aligned}&\langle\!\langle \alpha FM, (\beta GN)^{+} | \tilde{\Pi} | \alpha' F'M', (\beta' G'N')^{+} \rangle\!\rangle \\ &\quad = \delta - \langle \alpha FM | S_c | \alpha' F'M' \rangle \langle \beta GN | S_c | \beta' G'N' \rangle^{*}\, \delta_{M-N,\, M'-N'},\end{aligned} \tag{3.6}$$

where $\delta = \delta_{\alpha\alpha'}\, \delta_{\beta\beta'}\, \delta_{FF'}\, \delta_{GG'}\, \delta_{MM'}\, \delta_{NN'}$.

The matrix element in the irreducible basis is defined and given by

$$\begin{aligned}\tilde{\Pi}_q(kk') &\equiv \langle\!\langle \alpha F(\beta G)^{+}; kq | \tilde{\Pi} | \alpha' F'(\beta' G')^{+}; k'q \rangle\!\rangle \\ &= \sum_{MM'} (-)^{G+G'+M+M'} \langle FGM(q-M) | kq \rangle \langle F'G'M'(q-M') | k'q \rangle \\ &\qquad \times \langle\!\langle \alpha FM, (\beta GM-q)^{+} | \tilde{\Pi} | \alpha' F'M', (\beta' G'M'-q)^{+} \rangle\!\rangle.\end{aligned} \tag{3.7}$$

We assumed that there is no coherence among the different Zeeman multiplets and we put $\beta' G' = \alpha' F'$ for the initial level and $\beta G = \alpha F$ for the final level. As mentioned earlier we need to consider only density matrices with $\beta G = \alpha F$ due to the assumptions we made about our initial state. It is noted that in this z' system there can be Zeeman coherence, or non-zero density matrices, $\rho_{\alpha' F' M',\, \alpha' F' M'-q}$ with $q \neq 0$. Then, eq. (3.7) reduces to

$$\begin{aligned}\tilde{\Pi}_q(kk') &= \sum_{MM'} (-)^{F+F'+M+M'} \langle FFM(q-M) | kq \rangle \langle F'F'M'(q-M') | k'q \rangle \\ &\qquad \times \langle\!\langle FM, (FM-q)^{+} | \tilde{\Pi} | F'M', (F'M'-q)^{+} \rangle\!\rangle.\end{aligned} \tag{3.8}$$

Using eq. (3.6) in eq. (3.8) we have

$$\tilde{\Pi}_q(kk') = \sum_{MM'} (-)^{F+F'+M+M'} \langle FFM(q-M)\,|\,kq\rangle \langle F'F'M'(q-M')\,|\,k'q\rangle$$

$$\times [\delta_{\alpha\alpha'}\delta_{FF'}\delta_{MM'} - \langle \alpha FM|S_c|\alpha' F'M'\rangle \langle \alpha F(M-q)\,|S_c|\,\alpha' F'(M'-q)\rangle^*]. \tag{3.9}$$

Equation (3.4) is rewritten as

$$\mathrm{d}\tilde{\rho}^k{}_{q'}(F)/\mathrm{d}t = 2\pi n_p\, v \int [-\tilde{\Pi}_{q'}(kk')]\, b\, \mathrm{d}b\, \tilde{\rho}^{k'}{}_{q'}(F'). \tag{3.10}$$

We define the cross section by the formula,

$$\sigma_q(kk') = 2\pi \int [\pm \tilde{\Pi}_q(kk')]\ b\ \mathrm{d}b, \tag{3.11}$$

where the plus sign applies to the case of $\alpha F = \alpha' F'$ or "elastic" collisions, and the minus sign to $\alpha F \neq \alpha' F'$ or "inelastic" collisions. This convention is chosen for the convenience of expressing the rate equations which will be given later.

We now write down the cross section, eq. (3.11), from eq. (3.9). Let the integral cross section for transition from magnetic sublevel $\alpha' F'M'$ to magnetic sublevel αFM be $Q_{\alpha FM,\,\alpha' F'M'}$ which is defined by,

$$Q_{\alpha FM,\,\alpha' F'M'} = 2\pi \int |\langle \alpha FM|S_c|\alpha' F'M'\rangle|^2\ b\ \mathrm{d}b. \tag{3.12}$$

For excitation or deexcitation of $\alpha F \leftarrow \alpha' F'$ $(\alpha F \neq \alpha' F')$ we have

$$\sigma_0(00) = (2F+1)^{-1/2}(2F'+1)^{-1/2} \sum_{MM'} Q_{\alpha FM,\,\alpha' F'M'} \tag{3.13a}$$

$$\sigma_0(20) = (2F'+1)^{-1/2} \sum_{MM'} (-)^{F-M}\langle FFM-M|20\rangle\, Q_{\alpha FM,\,\alpha' F'M'} \tag{3.13b}$$

$$\sigma_0(02) = (2F+1)^{-1/2} \sum_{M'} (-)^{F'-M'} \langle F'F'M'-M'|20\rangle \sum_{M} Q_{\alpha FM,\,\alpha' F'M'} \tag{3.13c}$$

$$\sigma_0(22) = \sum_{MM'} (-)^{F+F'+M+M'} \langle FFM-M|20\rangle \langle F'F'M'-M'|20\rangle\, Q_{\alpha FM,\,\alpha' F'M'} \tag{3.13d}$$

and for $q = 1$ or 2 we have,

$$\sigma_q(22) = \sum_{MM'} (-)^{F+F'+M+M'} \langle FFM(q-M)|2q\rangle \langle F'F'M'(q-M')|2q\rangle$$

$$\times\ 2\pi \int \langle \alpha FM|S_c|\alpha' F'M'\rangle \langle \alpha F(M-q)|S_c|\alpha' F'(M'-q)\rangle^* \, b\, db. \qquad (3.13e)$$

It is to be noted that the coherence transfer cross section, eq. (3.13e), cannot be expressed in terms of the magnetic-sublevel-to-magnetic-sublevel cross sections.

We define the total cross section for depopulation from magnetic sublevel $\alpha FM'$ by inelastic collisions by the formula,

$$D_{\alpha FM'} = 2\pi \int \sum_M [\delta_{MM'} - |\langle \alpha FM|S_c|\alpha FM'\rangle|^2]\, b\, db. \qquad (3.14)$$

For "elastic" collisions of $\alpha F \leftarrow \alpha F$, the cross sections are given by,

$$\sigma_0(00) = (2F+1)^{-1} \sum_{M'} D_{\alpha FM'} \qquad (3.15a)$$

$$\sigma_0(20) = (2F+1)^{-1/2} \sum_{M'} (-)^{F-M'} \langle FFM'-M'|20\rangle D_{\alpha FM'}$$

$$+ (2F+1)^{-1/2} \sum_{M\neq M'} [(-)^{F-M'} \langle FFM'-M'|20\rangle - (-)^{F-M}\langle FFM-M|20\rangle]\, Q_{\alpha FM,\,\alpha FM'} \qquad (3.15b)$$

$$\sigma_0(02) = (2F+1)^{-1/2} \sum_{M'} (-)^{F-M'} \langle FFM'-M'|20\rangle D_{\alpha FM'} \qquad (3.15c)$$

$$\sigma_0(22) = \sum_{M'} \langle FFM'-M'|20\rangle^2 D_{\alpha FM'}$$

$$+ \sum_{M\neq M'} \langle FFM'-M'|20\rangle [\langle FFM'-M'|20\rangle - (-)^{M-M'} \langle FFM-M|20\rangle]\, Q_{\alpha FM,\,\alpha FM'} \qquad (3.15d)$$

and for $q = 1$ or 2 we have,

$$\sigma_q(22) = \sum_{MM'} (-)^{F+F'+M+M'} \langle FFM(q-M)|2q\rangle \langle F'F'M'(q-M')|2q\rangle$$

$$\times\ 2\pi \int [\delta_{MM'} - \langle \alpha FM|S_c|\alpha' F'M'\rangle \langle \alpha F(M-q)|S_c|\alpha' F'(M'-q)\rangle^*]\ b\, db. \qquad (3.15e)$$

3.2 *Axially symmetric distribution*

For the sake of simplicity of expressions we abbreviate eq. (3.10) to

$$d\tilde{\rho}^{k}{}_{q'}(F)/dt = -\tilde{g}_{q'}(kk')\,\tilde{\rho}^{k'}{}_{q'}(F'). \tag{3.10a}$$

Now we consider the situation in which the angular distribution of $\mathbf{v}$ is axially symmetric around the z-axis. The density matrix in the z-system is expressed as,

$$\rho^{k}{}_{q}(F) = \sum_{q'} R^{(k)}{}_{qq'}\,\tilde{\rho}^{k}{}_{q'}(F), \tag{3.16}$$

and the inverse transformation is,

$$\begin{aligned}\tilde{\rho}^{k}{}_{q'}(F) &= \sum_{q''} (R^{-1})^{(k)}{}_{q'q''}\,\rho^{k}{}_{q''}(F)\\ &= \sum_{q''} (-)^{q''-q'} R^{(k)}{}_{-q'',-q'}\,\rho^{k}{}_{q''}(F),\end{aligned} \tag{3.17}$$

where $R^{(k)}{}_{qq'}$ is the matrix for rotaion from the "z-system" to the "z'-system" with the Euler angle $(\phi, \theta, 0)$. The time development of the irreducible component in the z-system is given in terms of those in the z'-system as

$$\begin{aligned}d\rho^{k}{}_{q}(F)/dt &= -\sum_{q'} R^{(k)}{}_{qq'}\,\tilde{g}_{q'}(kk')\,\tilde{\rho}^{k'}{}_{q'}(F')\\ &= -\sum_{q'}\sum_{q''} (-)^{q''-q'} R^{(k)}{}_{qq'} R^{(k')}{}_{-q'',-q'}\,\tilde{g}_{q'}(kk')\,\rho^{k'}{}_{q''}(F')\\ &= -\sum_{q'}\sum_{q''}\sum_{K} (-)^{q''-q'} R^{(K)}{}_{q-q'',0}\,\langle kk'q\ -q''|K(q-q'')\rangle\langle kk'q'\ -q'|K0\rangle\\ &\qquad \times \tilde{g}_{q'}(kk')\,\rho^{k'}{}_{q''}(F').\end{aligned} \tag{3.18}$$

We now integrate the effects of collisions over ϕ. By using the relationship

$$R^{(K)}{}_{MM'}(\phi, \theta, \gamma) = e^{-i\phi M}\, r^{(K)}{}_{MM'}(\theta)\, e^{-i\gamma M'}, \tag{3.19}$$

and the fact that the velocity distribution of the perturbers is axially symmetric, we drop, on the right-hand side of eq. (3.18), the terms other than those for which $q'' = q$, to get,

$$\mathrm{d}\rho^{k}{}_{q}(F)/\mathrm{d}t = -2\pi \sum_{q'} (-)^{q-q'}\, \tilde{g}_{q'}(kk') \sum_{K} \langle kk'q\ -q|K0\rangle \langle kk'q'\ -q'|K0\rangle$$

$$\times\ R^{(K)}{}_{00}(0,\theta,0)\,\rho^{k'}{}_{q}(F'). \tag{3.20}$$

Let the velocity distribution function over the polar angle θ be $f_{v}(\theta)$. The integration over the angle leads to the following equation,

$$\mathrm{d}\rho^{k}{}_{q}(F)/\mathrm{d}t = -\ g_{q}(kk')\,\rho^{k'}{}_{q}(F'), \tag{3.21}$$

where we have defined $g_{q}(kk')$ as,

$$g_{q}(kk') = \sum_{q'} (-)^{q-q'}\, \tilde{g}_{q'}(kk') \sum_{K} \langle kk'q\ -q|K0\rangle \langle kk'q'\ -q'|K0\rangle$$

$$\times \int f_{v}(\theta)\ P_{K}(\cos\theta)\ \sin\theta\ \mathrm{d}\theta, \tag{3.22}$$

and where we have used the equality of the rotation matrix and the Legendre polynomial, and 2π has been absorbed into $f_{v}(\theta)$. This equation is nothing but eq. (4.42) of Omont (1977).

It is convenient to expand the velocity distribution in terms of Legendre polynomials,

$$f_{v}(\theta) = \sum_{K} f_{K}\ P_{K}(\cos\theta) \tag{3.23}$$

with

$$f_{K} = [(2K+1)/2] \int f_{v}(\theta) P_{K}(\cos\theta)\sin\theta\,\mathrm{d}\theta. \tag{3.24}$$

In the following discussion we restrict ourselves to the irreducible components with rank k and k' lower than 2, *i.e.*, the population and the alignment. As we have assumed there is no coherence among the magnetic sublevels in a level, *i.e.*, $q = 0$, so that the relaxation matrix elements $g_{q}(kk')$ with $q \neq 0$ are unnecessary. The matrix elements, given by eq. (3.22), are written as

$$
\left.
\begin{aligned}
g_0(00) &= \tilde{g}_0(00)\,2f_0 \\
g_0(20) &= \tilde{g}_0(20)\,2f_2/5 \\
g_0(02) &= \tilde{g}_0(02)\,2f_2/5 \\
g_0(22) &= \tilde{g}_0(22)\,[2f_0/5 + 4f_2/35 + 12f_4/105] \\
&\quad + \tilde{g}_1(22)\,[2f_0/5 + 2f_2/35 - 8f_4/105] \\
&\quad + \tilde{g}_2(22)\,[2f_0/5 - 4f_2/35 + 2f_4/105].
\end{aligned}
\right\}
\tag{3.25}
$$

4 Velocity distribution and rate equation

We consider situations in which the perturbers are not monoenergetic, but they have a velocity distribution over v; the distribution is expressed by $f(v, \theta)$, which is normalized as

$$
2\pi \int v^2\,\mathrm{d}v \int \sin\theta\,\mathrm{d}\theta\, f(v, \theta) = 1 \tag{4.1}
$$

where we have assumed axial symmetry. The distribution function $f_v(\theta)$ in eqs. (3.22, 23) is replaced by $f(v, \theta)$, and the moments of the distribution function f_K in eqs. (3.23–25) may be rewritten as $f_K(v)$.

4.1 Rate equation in the irreducible-component representation

We define the rate coefficients for transition $\alpha' F' \rightarrow \alpha F$ or $r \rightarrow p$ as,

$$
\left.
\begin{aligned}
c^{00}(r, p) &= \int \sigma_0(00; r, p)\,2f_0(v)\ v^3\mathrm{d}v \\
c^{20}(r, p) &= \int \sigma_0(20; r, p)\,2f_2(v)/5\ v^3\mathrm{d}v \\
c^{02}(r, p) &= \int \sigma_0(02; r, p)\,2f_2(v)/5\ v^3\mathrm{d}v \\
c^{22}(r, p) &= \int [\sigma_0(22; r, p) + \sigma_1(22; r, p) + \sigma_2(22; r, p)]\,2f_0(v)/5\ v^3\mathrm{d}v \\
&\quad + \int [2\sigma_0(22; r, p) + \sigma_1(22; r, p) - 2\sigma_2(22; r, p)]\,2f_2(v)/35\ v^3\mathrm{d}v \\
&\quad + \int [6\sigma_0(22; r, p) - 4\sigma_1(22; r, p) + \sigma_2(22; r, p)]\,2f_4(v)/105\ v^3\mathrm{d}v.
\end{aligned}
\right\}
\tag{4.2}
$$

Spontaneous radiative transition processes are isotropic, and we have only the two corresponding rates: for $r \rightarrow p$ $(p \neq r)$

$$
A^{00}(r, p) = (2F_r+1)^{1/2}(2F_p+1)^{-1/2}\,A(r, p) \tag{4.3a}
$$

$$
A^{22}(r, p) = (-)^{F_r+F_p+1}(2F_r+1)\left\{\begin{matrix} F_r & F_r & 2 \\ F_p & F_p & 1 \end{matrix}\right\}A(r, p), \tag{4.3d}
$$

where $A(p, r)$ is the usual Einstein A coefficient and $\{\quad\}$ is the 6-j symbol. For $p \to p$, equation (3.15a) and eq. (3.15d) suggest

$$A^{00}(p, p) = A^{22}(p, p) = \sum_{r} A(p, r), \tag{4.4}$$

where we have utilized the facts that all the magnetic sublevels have an equal radiative transition probability and that $\sum_{(M')} \langle FFM'-M' | 20 \rangle^2 = 1$.

We now construct a set of rate equations for the ensemble of atoms according to eq. (3.21). We assume that the collisional and radiative processes are additive. For "population" we have

$$\begin{aligned} d\rho^0{}_0(p)/dt = & \sum_{r \neq p} [c^{00}(r, p)\ n_p + A^{00}(r, p)]\ \rho^0{}_0(r) \\ & - [c^{00}(p, p)\ n_p + A^{00}(p, p)]\ \rho^0{}_0(p) \\ & + \sum_{r \neq p} c^{02}(r, p)\ n_p\ \rho^2{}_0(r) \\ & - c^{02}(p, p)\ n_p\ \rho^2{}_0(p) \end{aligned} \tag{4.5}$$

and for "alignment"

$$\begin{aligned} d\rho^2{}_0(p)/dt = & \sum_{r \neq p} c^{20}(r, p)\ n_p\ \rho^0{}_0(r) \\ & - c^{20}(p, p)\ n_p\ \rho^0{}_0(p) \\ & + \sum_{r \neq p} [c^{22}(r, p)\ n_p + A^{22}(r, p)]\ \rho^2{}_0(r) \\ & - [c^{22}(p, p)\ n_p + A^{22}(p, p)]\ \rho^2{}_0(p). \end{aligned} \tag{4.6}$$

4.2 Rate equation in the conventional representation

The population in a level, or Zeeman multiplet, p is usually written as $n(p)$, which is related to $\rho^0{}_0(p)$ as

$$n(p) = (2F_p+1)^{1/2}\ \rho^0{}_0(p). \tag{4.7}$$

When we use $n(p)$ in place of $\rho^0{}_0(p)$ in eqs. (4.5, 6) we have an alternative expression for the rate equations which is more straightforward in physical significance. We also use $a(p)$ in place of $\rho^2{}_0(p)$.

We redefine the cross sections. For excitation or deexcitation ($\alpha F \neq \alpha' F'$), instead of eqs. (3.13a–e), we have

$$Q_0(00) = (2F'+1)^{-1} \sum_{MM'} Q_{\alpha FM,\, \alpha' F' M'} \qquad (4.8a)$$

$$Q_0(20) = (2F'+1)^{-1} \sum_{MM'} (-)^{F-M} \langle FFM{-M}|20\rangle\, Q_{\alpha FM,\, \alpha' F' M'} \qquad (4.8b)$$

$$Q_0(02) = \sum_{M'} (-)^{F'-M'} \langle F'F'M'{-M'}|20\rangle \sum_{M} Q_{\alpha FM,\, \alpha' F' M'} \qquad (4.8c)$$

and for $q = 0$, 1 and 2

$$Q_q(22) = \sigma_q(22). \qquad (4.8de)$$

For "elastic" collisions ($\alpha F = \alpha' F'$), instead of eqs. (3.15a–e), we have

$$Q_0(00) = \sigma_0(00) \qquad (4.9a)$$

$$Q_0(20) = (2F+1)^{-1} \sum_{M'} (-)^{F-M'} \langle FFM'{-M'}|20\rangle D_{\alpha FM'}$$
$$+ (2F+1)^{-1} \sum_{M\neq M'} \left[(-)^{F-M'} \langle FFM'{-M'}|20\rangle - (-)^{F-M} \langle FFM{-M}|20\rangle\right] Q_{\alpha FM,\, \alpha FM'} \qquad (4.9b)$$

$$\sigma_0(02) = \sum_{M'} (-)^{F-M'} \langle FFM'{-M'}|20\rangle D_{\alpha FM'} \qquad (4.9c)$$

and for $q = 0$, 1 and 2 we obtain

$$Q_q(22) = \sigma_q(22). \qquad (4.9de)$$

We now replace the cross sections $\sigma_q(kk';r,p)$ in eq. (4.2) by the new cross sections $Q_q(kk';r,p)$ and obtain rate coefficients $C^{kk'}(r,p)$ instead of the $c^{kk'}(r,p)$. The "transition probability" $A^{00}(r,p)$ is replaced by $A(r,p)$, $A^{22}(r,p)$ will be given by eq. (4.3d), and $A^{00}(p,p)$ and $A^{22}(p,p)$ will be given by eq. (4.4) as bofore.

It is obvious from eq. (4.8a) that the rate coefficient $C^{00}(r,p)$ for population transfer is nothing but the usual rate coefficient for excitation or deexcitation, which may be written as $C(r,p)$. The replacement of $A^{00}(r,p)$ in eq. (4.5) by $A(r,p)$ means the same.

At this point, we include ionization explicitly, which is a kind of extention of the final state of excitation to the continuum states. We remember that the deexcitation cross section $D_{\alpha FM'}$ of eq. (3.14) includes the contribution from ionization.

Equations (4.9a) and (3.15a) shows that $C^{00}(p,p)$ is the depopulation rate coefficient by inelastic collisions averaged over the magnetic sublevels. This is nothing but the total depopulation rate coefficient, including ionization, in the conventional sense, *i.e.*,

$$C^{00}(p,p) = \sum_{r\neq p} C(p,r) + S(p), \tag{4.10}$$

where $S(p)$ is the ionization rate coefficient. We can write down the rate equations in the form, for population,

$$\begin{aligned} dn(p)/dt = & \sum_{r\neq p} [C(r,p)\ n_p + A(r,p)]\ n(r) \\ & - [\{\sum_{r\neq p} C(p,r) + S(p)\} n_p + \sum_{r\neq p} A(p,r)]\ n(p) \\ & + \sum_{r\neq p} C^{02}(r,p)\ n_p\ a(r) \\ & - C^{02}(p,p)\ n_p\ a(p) \end{aligned} \tag{4.11}$$

and for alignment,

$$\begin{aligned} da(p)/dt = & \sum_{r\neq p} C^{20}(r,p)\ n_p\ n(r) \\ & - C^{20}(p,p)\ n_p\ n(p) \\ & + \sum_{r\neq p} [C^{22}(r,p)\ n_p + A^{22}(r,p)]\ a(r) \end{aligned}$$

$$- [C^{22}(p,p)\ n_e + \sum_{r \neq p} A(p,r)]\ a(p). \qquad (4.12)$$

One should remember that the conventional excitation or deexcitation rate coefficient $C(r,p)$ is calculated with the assumption of statistical population distribution over the magnetic sublevels in the initial level r, or with $\rho^2{}_0(r) = 0$. The spontaneous transition probability $A(r,p)$ is independent of population distribution among the magnetic sublevels.

Equation (4.11), except for the last two lines on the right-hand side, is the conventional rate equation for population. The third line, as can be seen from eq. (4.8c) with (4.2), represents the production of population in this level from population imbalance, or alignment, in other levels. The last line is a correction term to the second line due to the presence of alignment and unequal depopulation rate (eq. (4.9c)) among the magnetic sublevels.

The first line on the right-hand side of eq. (4.12) represents the production of alignment in this level from population in other levels. The second line consists of two contributions as shown in eq. (4.9b); the first part corresponds to the production of alignment by unequal depopulation rates of the magnetic sublevels in this level, and the second part is the alignment production by elastic collisions. This latter contribution would vanish within the framework of the present assumption of rectilinear path for collisions. (Omont 1977, Petrashen *et al.* 1984) If this assumption is removed the principle of detailed balance no longer holds for the spatially anisotropic collisions (see eq. (4.2); the second moment of the velocity distribution is operative.), and this term may have a non-zero value (Dashevskaya and Nikitin, 1987). The third line corresponds to the transfer of alignment from other levels to this level. The last line represents the decay of alignment; the interpretation of the second term, the total radiative decay rate, is straightforward. The first, the collisional term, contains the three cross sections $Q_0(22)$, $Q_1(22)$ and $Q_2(22)$ as shown in eq. (4.2). The contributions from $Q_0(22)$ has a clear meaning as inferred from eq. (3.15d); the first term represents the decay of alignment owing to depopulation. The second term represents the decay of alignment by elastic collisions. This last process may be called *disalignment*.

It is to be noted that eqs. (4.11, 12) describe the kinetics of excited state atoms under the ionizing plasma environment, *i.e.*, the excited level population and alignment are created starting from the ground-state atoms (Fujimoto, 1979). We sometimes encounter situations where this assumption is not valid; Excited level population may be created starting from the ions through recombination. We call this situation a recombining plasma. In the present context, perturbers with an anisotropic velocity distribution may create aligned excited atoms. In the case that the perturbers are neutral atoms anisotropic charge exchange recombination collisions may create aligned 'atoms'. Electrons with anisotropic velocity distribution could recombine with the ions through radiative recombination, three body recombination, or even dielectronic recombination. We could incorprate these contributions into eqs. (4.11, 12). As its result the population and the alignment in excited levels have two components, namely the ionizing plasma component and the recombining plasma component. (Fujimoto 1979, 1980) The former is proportional the the ground-state population and the latter is proportional to the ion density. The present formalism, eqs. (4.11, 12) is for the ionizing plasma component of population and alignment.

4.3 Cross sections and polarization

Let r be the initial state and p the final state of atoms which are assumed to be at rest. We consider population transfer or excitation/dexcitation $r \rightarrow p$ of these atoms by a monoenergetic beam of particles having velocity v_0 in the z-direction. From eq. (3.24) we have the expansion coefficient of the velocity distribution function

$$f_0(v) = \delta(v-v_0)/2v_0^2$$
$$f_2(v) = 5\delta(v-v_0)/2v_0^2. \tag{4.13}$$

Equation (4.11) reduces in this case to

$$dn(p)/dt = C(r,p)\ n(r)\ n_P$$

$$= Q_0(00;r,p)\ v_0\ n(r)\ n_P \tag{4.14}$$

where we have used the first line of eq. (4.2), with $\sigma_0(00;r,p)$ replaced by

$Q_0(00;r,p)$, and eq. (4.13).

We now consider alignment production in level p by excitation/deexcitation $r \to p$; then equation (4.2) reduces to

$$da(p)/dt = C^{20}(r,p)\ n(r)\ n_p$$

$$= Q_0(20;r,p)\ v_0\ n(r)\ n_p \qquad (4.15)$$

where we have used the second line of eq. (4.2), with $\sigma_0(20;r,p)$ replaced by $Q_0(20;r,p)$ and eq. (4.13).

Suppose we observe an emission line for transition $p \to s$ from the direction perpendicular to the beam direction with the polarized components resolved. The longitudinal alignment is defined as

$$A_L(p,s) = (I_{//} - I_{\perp})/(I_{//} + 2I_{\perp}) \qquad (4.16)$$

where $I_{//}$ and $I_{\perp}$ are the intensity of the polarized component with its polarization direction in the beam direction and that with perpendicular to it, respectively. It can be expressed in terms of the irreducible components of the upper level atoms in the form, (Omont 1977)

$$A_L(p,s) = (-)^{F_p+F_s}\sqrt{3/2}\ (2F_p+1)\begin{Bmatrix} F_p & F_p & 2 \\ 1 & 1 & F_s \end{Bmatrix}\ a(p)/n(p) \qquad (4.17)$$

From the comparison of this equation with eqs. (4.14), and (4.15), we may express the alignment production cross section in terms of the experimentally determined longitudinal alignment and the excitation cross section as

$$Q_0(20;r,p) = (-)^{F_p+F_s}\sqrt{2/3}\ (2F_p+1)^{-1}\begin{Bmatrix} F_p & F_p & 2 \\ 1 & 1 & F_s \end{Bmatrix}^{-1} A_L(p,s)\ Q_0(00;r,p) \qquad (4.18)$$

5 Example

For the purpose of demonstrating how to apply the present formulation to actual situations we treat as an example berylliumlike oxygen ions excited by electrons with an anisotropic velocity distribution in plasma. In this example since we start with the cross sections between the magnetic sublevels for our rate equations, the final results of the present development, which, at the start, was based on the semi-classical approximation, is appropriate. We consider levels $2s^2\ {}^1S_0$, $2s2p\ {}^3P_{0,1,2}$, $2s3p\ {}^3P_{0,1,2}$ and $2s3s\ {}^3S_1$. For transitions among these levels except for the last one, we have calculated excitation cross section between the magnetic sublevels $Q_{pM,rM'}$ by the distorted wave approximation. The formulas that we obtain in the quantum-mechanical formulation for $Q_0(00)$, $Q_0(20)$, and for $Q_0(02)$ are the same as what we obtained in the semi-classical formulation (given by eqs. (4.8a, b, c)). Figure 1 shows examples of the cross sections for transition $2s2p\ {}^3P_1(M') \rightarrow 2s3p\ {}^3P_1(M)$ for $M' = 0$ or 1 and $M = 0$ or 1. According to eq. (4.8) the cross sections $Q_0(00;r,p)$, $Q_0(20;r,p)$, $Q_0(02;r,p)$ and $Q_0(22;r,p)$ are calculated. Figure 2 shows examples.

In this example, we consider only the cross sections discussed above, and neglect the others, *e.g.*, $Q_q(22;r,p)$ with $q = 1$ or 2, and $Q_0(20;p,p)$. We also neglected deexcitation. The radiative transition probability $A^{22}(r,p)$ is calculated from eq. (4.3d).

As an example of velocity distributions of electrons, we consider a Maxwellian distribution for the bulk electrons accompanied by a component having a shifted Maxwellian distribution. Figure 3 shows schematically the contour diagram of this distribution. We assume the number density and the temperature of the bulk electrons to be $3.8 \times 10^{18}\ \mathrm{m}^{-3}$ and 100 eV, respectively. Those of the shifted component are $1.2 \times 10^{18}\ \mathrm{m}^{-3}$ and 100 eV. The speed of the central velocity of the shifted component is varied. This distribution is axially symmetric around the z-axis. This velocity distribution over the polar angle is expanded in terms of the Legendre polynomials according to eq. (3.24). Figure 4a shows the even moments of the expansion coefficients. In our rate equation we use the expansion coefficient multiplied by v^3 as seen in eq. (4.2). Figure 4b shows these quantities. By multiplying the cross sections shown in Fig. 2 by the velocity distribution in Fig. 4b, we obtain the rate coefficients to be used in eqs. (4.11) and (4.12).

We first construct the rate equations for population, eq. (4.11). In this case we neglect the contributions from alignment, the third and fouth lines. This is justified because, as will be seen later, the relative magnitude of the alignment to the population is rather small, typically in the order of a percent. By the method of the collisional-radiative model, or by putting $d/dt = 0$ for the rate equation except for that for the ground state, we solve the set of the equations, obtaining the excited-level populations. We then substitute these solutions into the rate equation for alignment, eq. (4.12). By the similar procedure to that for population, we obtain the alignment for levels with F or $J \neq 0$. Figure 5 shows examples of the calculated $a(p)/n(p)$ for $2s2p\ ^3P_J$ and $2s3p\ ^3P_J$ for $J = 1$ and 2. We finally calculate the longitudinal alignment for emission lines according to eq. (4.17).

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Figure captions

Fig. 1. Magnetic-sublevel to magnetic-sublevel excitation cross sections for OV $2s2p\ {}^3P_1(M') \rightarrow 2s3p\ {}^3P_1(M)$ for $M' = 0$ or 1 and $M = 0$ or 1.

Fig. 2. $Q_0(00;r,p)$, $Q_0(20;r,p)$, $Q_0(02;r,p)$ and $Q_0(22;r,p)$ for OV $2s2p\ {}^3P_1 \rightarrow 2s3p\ {}^3P_1$.

Fig. 3. Schematic contour diagram of the velocity distribution of electrons with the bulk Maxwellian distribution with a shifted Maxwellian component.

Fig. 4. a. Even moments of the expansion coefficient of the velocity distribution. b. Those multiplied by v^3. The speed of the central velocity of the shifted component is assumed to be 1×10^7 m/s.

Fig. 5. Relative alignment, $\rho^2{}_0(p)/n(p)$, for $p = 2s2p\ {}^3P_J$ and $2s3p\ {}^3P_J$ with $J = 1$ or 2.

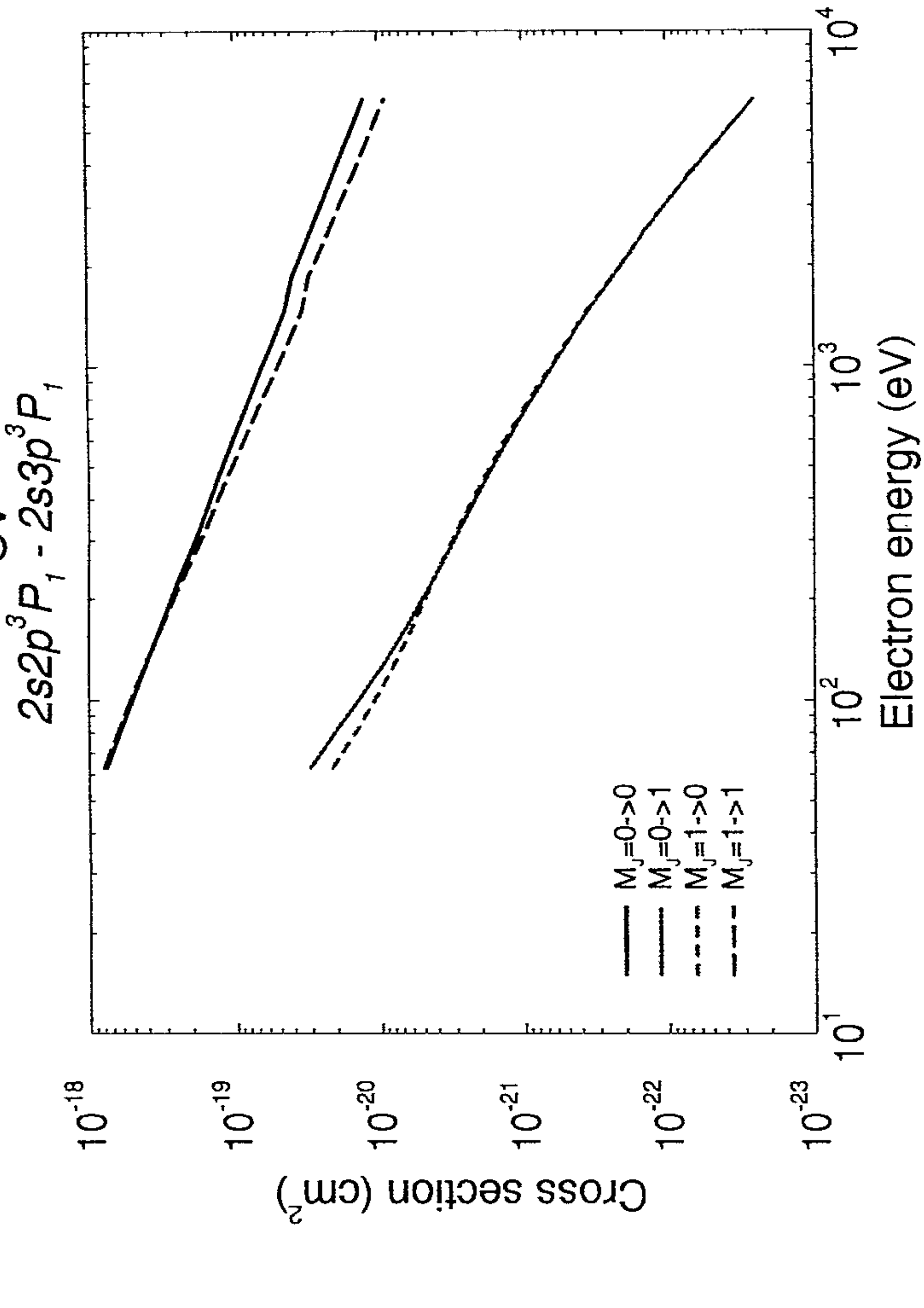
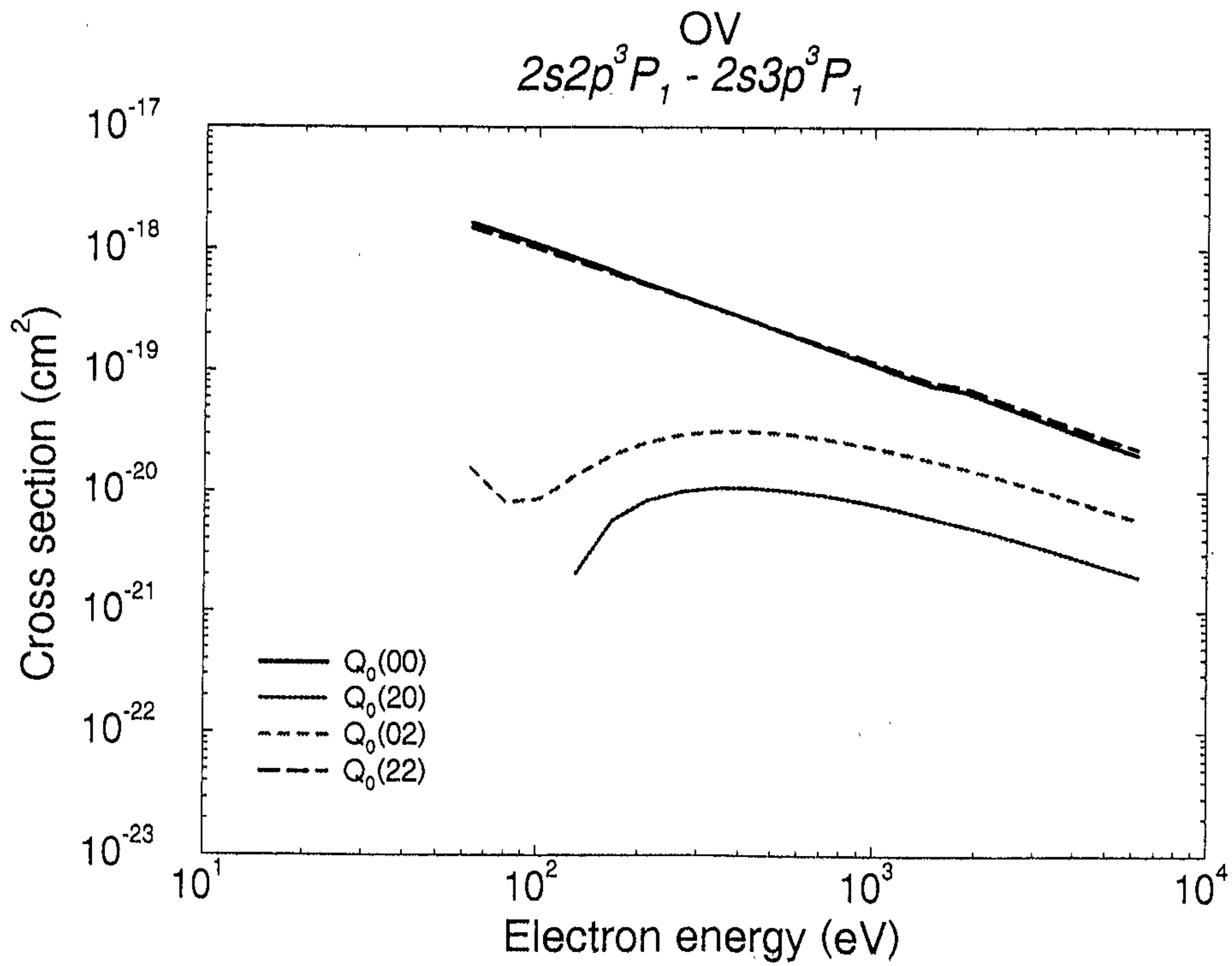

OV
2s2p3P1 - 2s3p3P1
Cross section (cm2)
10-18
10-19
10-20
10-21
10-22
10-23
101
102
103
104
Electron energy (eV)
MJ=0->0
MJ=0->1
MJ=1->0
MJ=1->1

Fig. 1



OV
2s2p³P₁ - 2s3p³P₁
Cross section (cm²)
Electron energy (eV)
Q₀(00)
Q₀(20)
Q₀(02)
Q₀(22)

Fig. 2

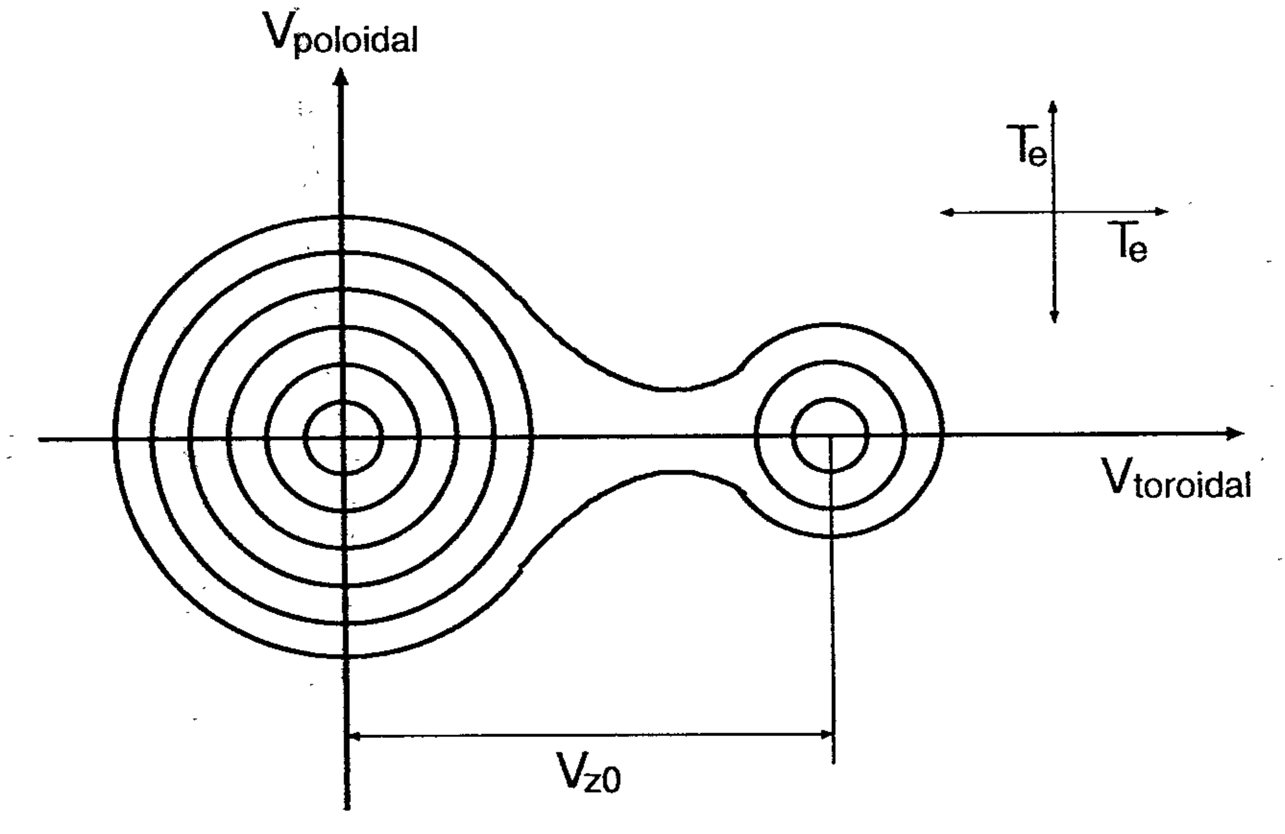
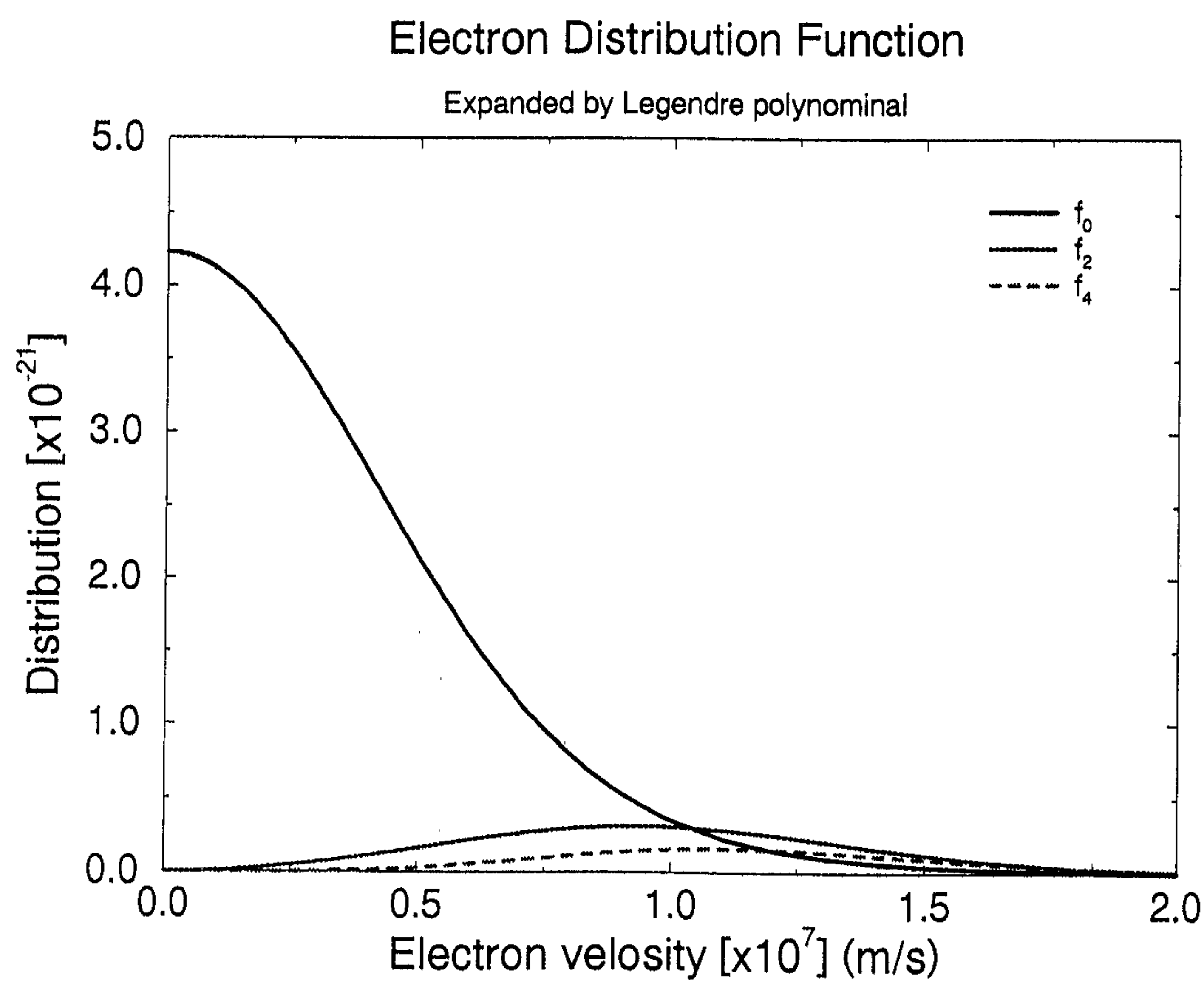
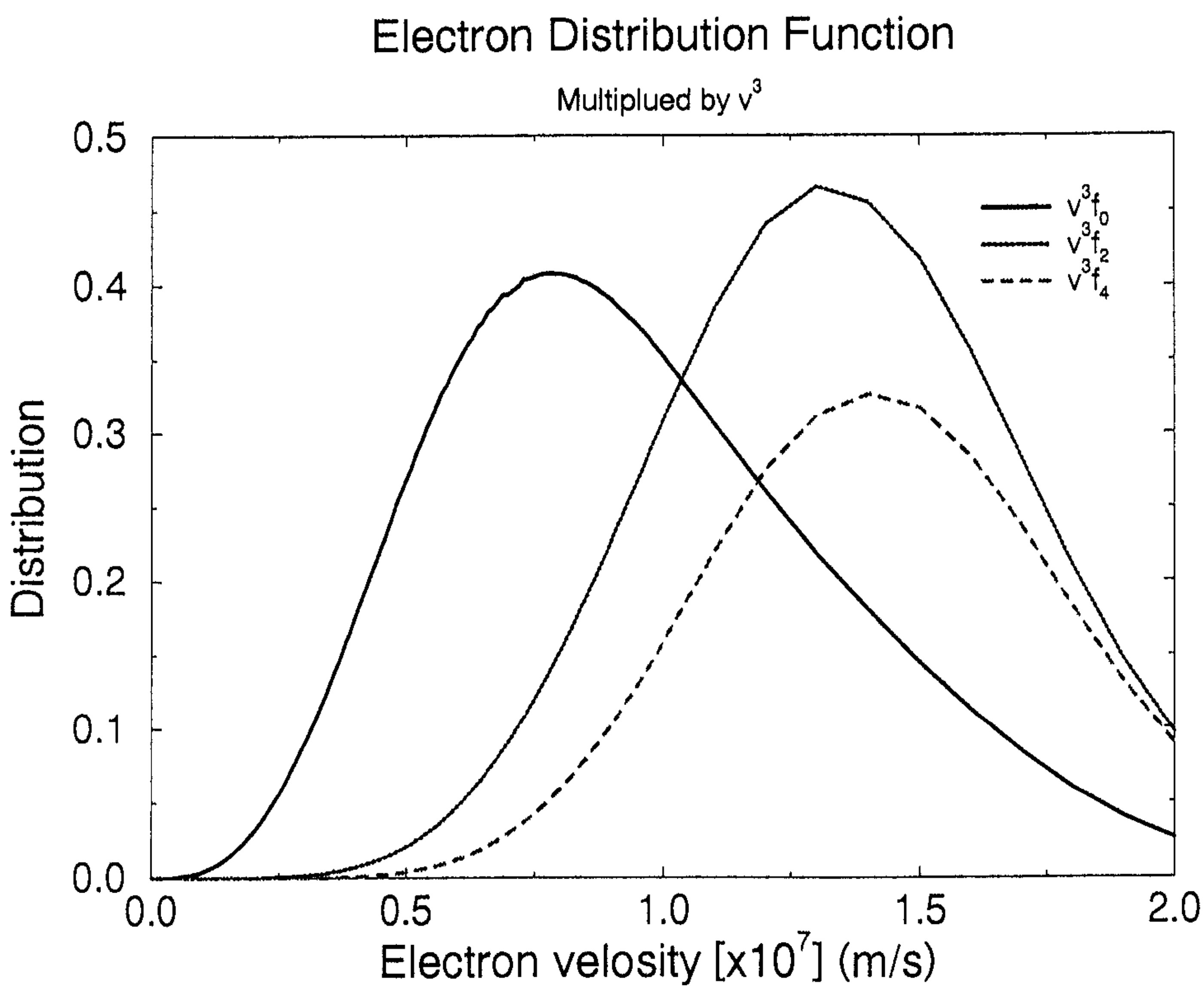


Fig. 3.



Electron Distribution Function
Expanded by Legendre polynominal
5.0
4.0
3.0
2.0
1.0
0.0
Distribution [x10^-21]
0.0
0.5
1.0
1.5
2.0
Electron velosity [x10^7] (m/s)
f0
f2
f4

Fig. 4a



Electron Distribution Function
Multiplued by v3
0.5
0.4
0.3
0.2
0.1
0.0
Distribution
v3f0
v3f2
v3f4
0.0
0.5
1.0
1.5
2.0
Electron velosity [x107] (m/s)

Fig. 4b

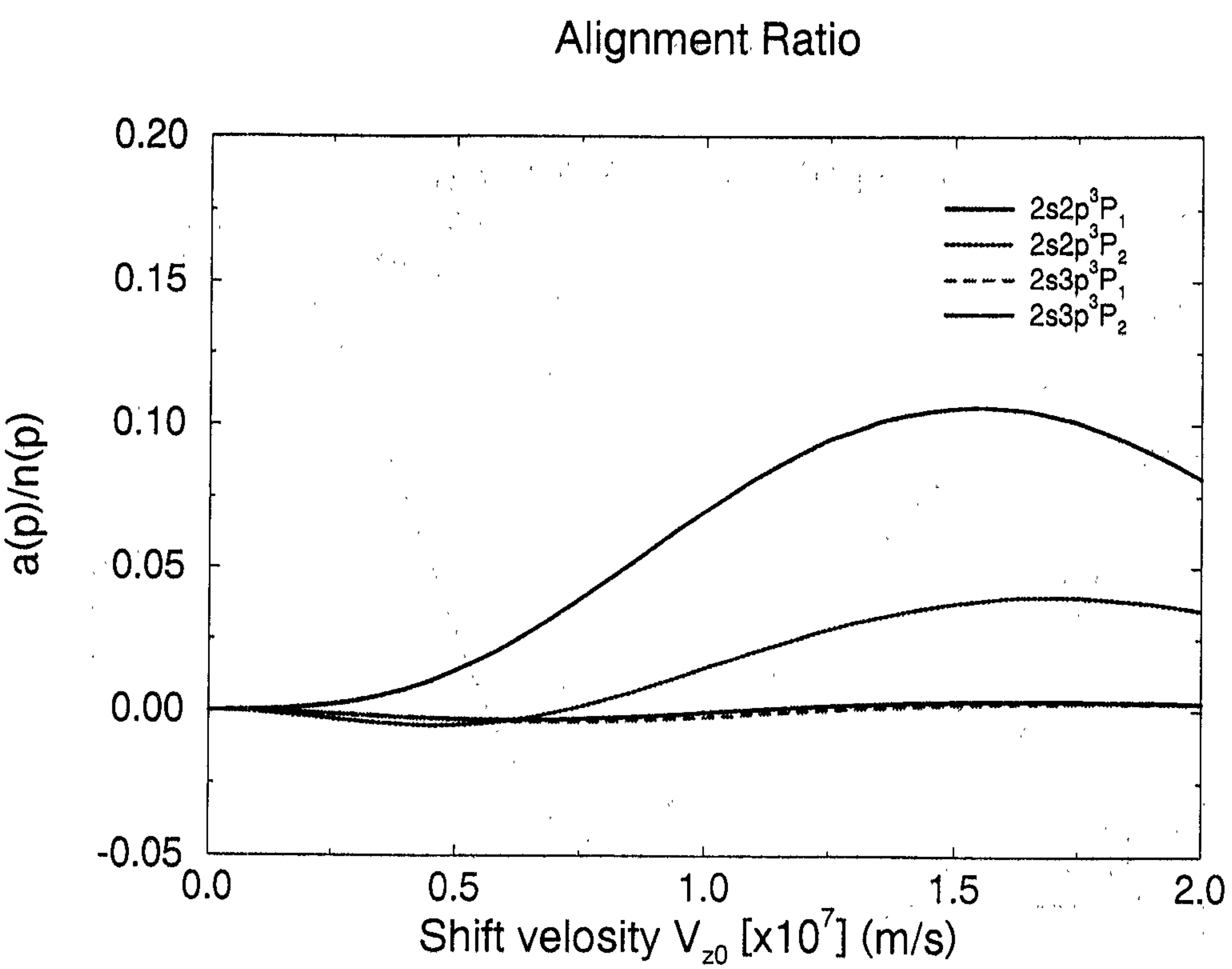

Alignment Ratio
0.20
0.15
0.10
0.05
0.00
-0.05
a(p)/n(p)
0.0
0.5
1.0
1.5
2.0
Shift velosity V_{z0} [x10^7] (m/s)
2s2p $^3P_1$
2s2p $^3P_2$
2s3p $^3P_1$
2s3p $^3P_2$

Fig. 5

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