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Di-electronic recombination of He-like ions: Fe^{24+}

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Abstract. A fast reliable method is described for the calculation of the total di-electronic recombination rate coefficient $\alpha_d(i; \text{tot})$ of a ground-state He-like ion i. The equivalent-electron frozen-core approximation of Badnell is used to describe the three-electron problem. Electron exchange in the radial function of the spectator electron is allowed for by using the CEDW radial equations of Badnell. A very accurate result for the total di-electronic recombination rate coefficient for a highly charged ion can be obtained from a single-configuration LS-coupling calculation if $A_a \ll A_r$ and $\bar{A}_a \ll \bar{A}_r$, where $U: A_i \rightarrow \bar{A}_i$, since this implies that $\alpha_d(i; \text{tot})$ remains almost unchanged under the unitary transformation U to configuration mixing and intermediate coupling.

For Fe^{24+}, di-electronic recombination via intermediate states of the form $1sn_cl_cnl$ has been calculated directly for $2 \leqslant n_c \leqslant n \leqslant 5$ and $\forall l_c, l$. Tables of a small set of reuslts that depend only on n_c and n are presented. The contribution from higher states ($n > 5$, $2 \leqslant n_c \leqslant 5$) is estimated by downward extrapolation of the excitation partial collision strengths of Badnell and also by upward extrapolation using the n^{-3} asymptotic dependence of A_a. The results obtained for $n_c = 2$ with $2 \leqslant n \leqslant 4$ are in excellent agreement (5% and better) with those derived from the configuration-mixing intermediate-coupling satellite intensities of Bely-Dubau *et al.* It is shown that the estimate of Bely-Dubau *et al*, which is only for satellites to the $n_c = 2$ resonance line, forms only approximately 75% of the total di-electronic recombination rate coefficient and not 90% as they claimed. Results are presented for the total di-electronic recombination rate coefficient of the ground-state Fe^{24+} ion; the results of the general formula of Burgess are approximately 30% higher.

1. Introduction

The process of resonant capture

$$X^{(Z)+}(i) + e^-(E, l') \rightleftharpoons X^{(Z-1)+}(j, nl) \tag{1.1}$$

followed by radiative stabilisation

$$X^{(Z-1)+}(j, nl) \rightarrow X^{(Z-1)+}(k, nl) + h\nu \tag{1.2}$$

di-electronic recombination (see Massey and Bates 1942-3), was invoked by Burgess (1964) to help resolve the discrepancy between the temperatures of the solar corona as deduced from observed linewidths and from ionisation balance calculations (see Burgess and Seaton 1964). The dominant contribution to the above process comes from large values of nl for the coronal ions used in those calculations (see Burgess 1965a, 1966), allowing the simple technique of extrapolation of excitation partial collision strengths to be used in the calculation of the di-electronic recombination rate

coefficient $\alpha_d(i;\text{tot})$. This approach can be unreliable when $\alpha_d(i;\text{tot})$ is dominated by capture to low n states, for example, in the case of He-like and H-like ions (see § 2.1).

The $n=2$ Li-like lines (1.2 with $k=1s^2$ and $j=1sn_cl_c$) were first observed as satellites to the He-like resonance line by Edlén and Tyrén (1939). Later observations in laboratory and astrophysical plasmas stimulated their classification (by Gabriel and Jordan 1969) and their theoretical description (see Gabriel and Paget 1972, Gabriel 1972, Bhalla *et al* 1975). The use of satellite-to-resonance intensity ratios as a plasma diagnostic (see Gabriel and Jordan 1972) has led to much work being done on the calculation of He-like satellite intensities (see Dubau and Volonté (1980) for a general review).

The total di-electronic recombination rate, just being equal to the sum of all the satellite intensities of all the resonance lines, provides (in theory) another approach to the calculation of $\alpha_d(i;\text{tot})$. Bely-Dubau *et al* (1979a, b) have calculated directly the intensities of the $n=2$, 3 and 4 satellites to the $n_c=2$ resonance line for Fe^{24+} with configuration mixing and intermediate coupling, and have extrapolated these results upwards to estimate the contribution from higher satellites. Similar satellite intensities have been calculated for Ca^{18+} and Ti^{20+} by Bely-Dubau *et al* (1982a, b) and for Mg^{10+} by Steenman-Clark *et al* (1980). As Z decreases a larger number of levels start to contribute to $\alpha_d(i;\text{tot})$ making reliable calculations more difficult. However, Bely-Dubau *et al* (1981) have calculated the intensity of satellites to the $n_c=2$ resonance line of O^{6+} for $n=2$ to 5 and provide an estimate for $n=6$.

A similar approach can be used to provide an experimental estimate of $\alpha_d(i;\text{tot})$, namely by summing over the observed satellite-to-resonance intensity ratios and multiplying by the excitation rate coefficient for the resonance transition. Observations have been made (for $n_c=2$ and $n=2$ and 3 only) for Ca^{18+} and Ti^{20+} by Chichkov *et al* (1981), for Fe^{24+} by Bitter *et al* (1979, 1981, see also Bely-Dubau *et al* 1983) and for Mg^{10+} to K^{17+} by Boiko *et al* (1978).

The main interest in satellite intensities has been as a plasma diagnostic and consequently great accuracy is required of each individual satellite which is not necessarily relevant to the calculation of the total di-electronic recombination rate coefficient. Estimates of the di-electronic recombination rate coefficient from satellite intensities have only included the contribution from the $n_c=2$ resonance line, which is the dominant contribution (about 75% of the total). However, in this paper we also investigate the contribution from $n_c>2$ resonance lines.

We note that Nasser and Hahn (1983) have calculated di-electronic recombination rates for O^{6+}, Ar^{16+}, Fe^{24+} and Mo^{40+} using an angular-momentum-averaged scheme. This simplified procedure is used to calculate the contribution from all possible intermediate states, from which a dominant subset is then selected and recalculated in single-configuration *LS* coupling. Their final result is obtained after scaling the *LS*-coupling results so as to take account of the states not included in the *LS*-coupling subset.

We now draw together the threads of a recent series of papers to provide a fast reliable method for the calculation of total di-electronic recombination rate coefficients for He-like ions. We use the equivalent-electron frozen-core approximation of Badnell (1984, hereafter referred to as III) to describe the three-electron problem. We allow for electron exchange in the radial function of the *nl* spectator electron by using the CEDW approximations of Badnell (1983a, b, hereafter referred to as I and II respectively). We calculate $\alpha_d(1s^2;1sn_cl_cnl)$ directly for $2\leqslant n_c\leqslant n\leqslant 5$ and $\forall l_c$, l as described in § 2. The contribution from higher satellites ($n>5$, $2\leqslant n_c\leqslant 5$) is estimated in two

ways: firstly by extrapolation downwards from the continuum of the excitation partial collision strengths of Badnell (1985, hereafter referred to as IV) and secondly by upward extrapolation using the asymptotic n^{-3} dependence of A_a. In § 3 we compare our results for Fe^{24+} with those obtained from the general formula (GF) of Burgess (1965b) and, where possible, with the experimental and theoretical results that were obtained by other workers by summing satellite intensities.

2. Theory

The theory of di-electronic recombination and the calculation of di-electronic recombination rates have been reviewed by Seaton and Storey (1976). Since then Bell and Seaton (1985) have developed an *ab initio* theory for di-electronic recombination making use of quantum defect theory (see Seaton 1983), and the generalised radiation-damping theory of Davies and Seaton (1969) to allow for overlapping resonances and their interaction with the radiation field. However, they find that for plasma conditions their results for total di-electronic recombination rates differ little from those obtained using the intuitive approach of Burgess (1964, 1966).

2.1. The di-electronic recombination rate coefficient

Following Burgess (1965a, 1966) and in his notation, using detailed balance arguments and the Saha equation for thermodymamic equilibrium, the di-electronic recombination rate coefficient for a given initial state i and an intermediate state (j, nl) is given by

$$\alpha_d(i; j, nl) = \left(\frac{4\pi a_0^2 I_H}{k_b T}\right)^{3/2} \sum_k [A_r(j, nl \to k, nl) + A_r(j(n_c l_c), nl \to k, n_c l_c)] \times \frac{\omega(j, nl)}{2\omega(i)} b(j, nl) \exp(-E/k_b T) \tag{2.1}$$

where E is the energy (in Rydbergs) of the continuum electron, which is fixed by the position of the resonances, and

$$b(j, nl) = \frac{\Sigma_{l'} A_a(j, nl \to i, El')}{\Sigma_k [A_r(j, nl \to k, nl) + A_r(j(n_c l_c), nl \to k, n_c l_c) + \Sigma_{l'} A_a(j, nl \to k, El')]} \tag{2.2}$$

$$\left(\frac{4\pi a_0^2 I_H}{k_b}\right)^{3/2} = 4.1414 \times 10^{-16} \text{ cm}^3.$$

We note that we have allowed for the possibility of the spectator electron radiating in (2.1) and (2.2). The total di-electronic recombination rate coefficient for a given initial state i is given by

$$\alpha_d(i; \text{tot}) = \sum_{j,nl} \alpha_d(i; j, nl). \tag{2.3}$$

The approach of Burgess (1964, 1965b) to the calculation of $\alpha_d(i; j, nl)$ is to evaluate $b(j, nl)$ in the Coulomb-Bethe approximation and then to multiply the A_a by a correction factor, this factor being the ratio of the best available excitation partial collision strengths (eg CEDW2 or CEDW3) to those of the Coulomb-Bethe approximation, extrapolated from just above to below threshold. $\alpha_d(i; j, nl)$ is then evaluated from

(2.1) with $A_r(j(n_c l_c), nl \to k, n_c l_c) = 0$ and $A_r(j, nl \to k, nl) = A_r(j \to k)$, using the best available value for $A_r(j \to k)$. We introduce additionally a correction factor for $A_r(j \to k)$ in $b(j, nl)$, this factor being the ratio of the $A_r(j \to k)$ used in (2.1) to that of the Coulomb-Bethe approximation.

This approach works well in general for $\Delta n_c = 0$ core transitions since the dominant contribution to $\Sigma_{nl} b(j, nl)$ comes from large values of n (see, for example, Burgess 1965a, 1966 figure 1) where $A_a \gg A_r$ and so α_d is relatively insensitive to errors in A_a. However, for He-like ions ($\Delta n_c \geq 1$) $\Sigma_{nl} b(j, nl)$ is dominated by capture to low n states (see figure 2 of Burgess and Tworkowski (1976) which is for the similar case of H-like ions) and exchange effects can be expected to be important here. In this case A_r scales as Z^4 and A_a is independent of Z, to first order, and so for Z large enough $A_a \ll A_r \forall n$ and α_d is sensitive to errors in A_a. In particular, the operation of the Pauli exclusion principle means that the extrapolation method is unreliable for $n_c = n$. Thus we solve directly for the $n_c = n$ (and higher) levels as described in the following sections.

In (2.1) and (2.2) $n \to 1$ radiative transitions dominate $\Sigma_k A_r(j \to k)$ due to their large energy difference and so setting $k = i$ can be expected to have a negligible effect on $\alpha_d(i; \text{tot})$. In (2.2) $\Sigma_k A_a(j \to k)$ contains rates for transitions back into the continuum of the ground configuration ($k = i$) as well as into the continuum of excited configurations ($k \neq i$). The $\Delta n_c = 0$ core transitions $A_a(1s n_c l_c nl \to 1s n_c l'_c El')$ can be expected to dominate the $\Delta n_c \neq 0$ transitions $A_a(1s n_c l_c nl \to 1s^2 El')$ and thus suppress di-electronic recombination via $\Delta n_c \neq 0$ core transitions. Thus we impose an upper limit n_0 on the sum over n in (2.3) determined by the lowest value of n for which the $\Delta n_c = 0$ Auger transition is energetically possible. However, for a highly charged ion any error due to this cut-off has little effect on $\alpha_d(i; \text{tot})$; for Fe^{24+}, less than 1% of $\alpha_d(i; \text{tot})$ could come from $n > n_0$ ($n_0 = 15$ using $\Delta E(2^1P - 2^1S)$ of Fuhr *et al* 1981). A $\Delta n_c \neq 0$ core transition $A_a(1s n_c l_c nl \to 1s n'_c l'_c El')$ into the continuum of an excited configuration is energetically possible for a much lower vaue of n, in fact $\forall n > n_c$ for $n_c = 3$ and 4 for Fe^{24+}. However, $\Sigma_k A_a(j \to k) \ll A_r(j \to i) \forall n > n_c$ still and so negligible error will arise on setting $k = i$, particularly as for Fe^{24+} at most 5% of $\alpha_d(i; \text{tot})$ is affected by this process. In other words, for a highly charged ion, after a $\Delta n_c \neq 0$ radiationless capture has taken place the system radiatively stabilises before it has time to auto-ionise (via $\Delta n_c \neq 0$) either back into the original continuum or into a new one.

We conclude that for a highly charged He-like ion it is a good approximation to consider only $k = i$ in the evaluation of $\alpha_d(i; \text{tot})$.

2.2. Autoionisation transition rates

The autoionisation transition probability rate A_a is given in first-order perturbation theory by (see, for example, Cowan 1981)

$$A_a(t' \to t) = \left(\frac{8 I_H}{\hbar}\right) |\langle t|H|t'\rangle|^2 \tag{2.4}$$

$$= \frac{I_H}{\hbar} \frac{\Omega^I_B(t, t')}{\omega(t)} \tag{2.5}$$

where $\omega(t) = \omega(t')$, $I_H/\hbar = 2.06707 \times 10^{16}\ s^{-1}$ and $t = CSLp$, where C denotes a configuration and p the parity—which is conserved. The Hamiltonian H is given by equation (2.1) of III and the normalisation of the continuum radial function is given

by

$$\int_0^\infty F_{kl}F_{k'l}\,\mathrm{d}r = \pi\delta(k^2-k'^2). \tag{2.6}$$

For a He-like ion plus electron we consider (for $nl \neq n_c l_c$)

$$1s^2(^1S)kl'\,^2L' \rightleftharpoons 1sn_cl_c(^wL_c)nl\,^2L'$$

where $k^2 = E$ (the energy of the continuum electron) and $w = 2s_c+1$ denotes the spin multiplicity of the parent. Using the equivalent-electron frozen-core approximation and the three-electron wavefunction of III, we obtain for $\langle t|H|t'\rangle$

$$\langle 1sn_cl_c(^wL_c)nl\,^2L'|H|1s^2(^1S)kl'\,^2L'\rangle$$

$$= {}^wN^{-1/2}\Big[\, b_w f_{l_c}(0l', l_cl; l')R^l(1s, kl'; n_cl_c, nl) + h_w g_l(0l', l_cl; l')$$

$$\times\left(R^l(1s, kl'; nl, n_cl_c) - \tfrac{1}{2}\delta_{l_cl'}\delta_{l0}(\varepsilon_{1s}+\varepsilon_{n_cl_c})\int_0^\infty P_{1s}F_{ns}\,\mathrm{d}r\int_0^\infty P_{n_cl_c}F_{kl'}\,\mathrm{d}r\right)\Big]$$

where the Slater integral R^λ is given by (2.7)

$$R^\lambda(1s, kl'; n_cl_c, nl) = \int_0^\infty y_\lambda(P_{1s}, P_{n_cl_c})F_{kl'}F_{nl}\,\mathrm{d}r. \tag{2.8}$$

The normalisation coefficient ${}^wN$ is given by

$${}^wN = 1 - \tfrac{1}{2}(-1)^{s_c}\delta_{ll_c}\left(\int_0^\infty P_{n_cl_c}F_{nl}\,\mathrm{d}r\right)^2 \tag{2.9}$$

and

$$b_1 = 2^{1/2} \qquad h_1 = -2^{-1/2} \qquad b_3 = 0 \qquad h_3 = (3/2)^{1/2}. \tag{2.10}$$

We note that the notation used here suppresses the explicit dependence of F on P. P satisfies equation (2.15) of III which results from a Hartree frozen-core approximation. F satisfies one of the CEDW radial equations of I or III. The CEDW3 radial equation includes the lowest multipole exchange potential exactly and is thus the same as the equation obtained in an LS-determined Hartree–Fock frozen-core approximation when the multipole expansion contains a single term.

For the case of equivalent electrons ($nl = n_cl_c$) we consider

$$1s^2(^1S)kl'\,^2L' \rightleftharpoons 1s(^2S)nl^2(^wL')^2L'$$

where ${}^wL' = {}^1S, {}^1D, \ldots$ and we note that ${}^wL' = {}^3P, {}^3F, \ldots$ is forbidden by parity conservation. In this case of equivalent electrons we can no longer freeze one orbital and vary the other (i.e. equations (2.15) and (A1) of III are no longer valid) but must vary both, as discussed in I, to obtain (in the notation of III) the following LS-determined Hartree–Fock equation for the nl^2 orbital:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} + \frac{2Z}{r} - {}^{FC}V(r) - \sum_\lambda 2f_\lambda(ll, ll; L)y_\lambda(P_{nl}, P_{nl}) - \varepsilon_{nl}\right)P_{nl} = 0 \tag{2.11}$$

where

$$E_{TOT} = -2\varepsilon_{nl} - \sum_\lambda F^\lambda_{nl} - \varepsilon_c - F^0_c \tag{2.12}$$

is the total energy of the three-electron system and $\Sigma_\lambda F^\lambda_{nl}$ is the nl^2 interaction energy

given by

$$\sum_{\lambda} F^{\lambda}_{nl} = \sum_{\lambda} 2f_{\lambda}(ll, ll; L) R^{\lambda}(nl, nl; nl, nl). \tag{2.13}$$

We note that (2.13) averaged over *LS* gives the average Coulomb energy of an (equivalent) electron pair, in agreement with Cowan (1981 table 6-1). Equation (2.11) is non-linear and we solve it by iteration using an unperturbed *nl* orbital to start off with. $\langle t|H|t'\rangle$ is then given by

$$\begin{aligned}\langle 1s(^2S)nl^2(^wL')^2L'|H|1s^2(^1S)kl'^2L'\rangle &= f_l(0l', ll; l')R^l(1s, kl'; nl, nl) \\ &+ \delta_{l0}\int_0^{\infty} P_{1s}P_{ns}\,dr\left(\int_0^{\infty} y_0(P_{ns}P_{ns})P_{ns}F_{ks}\,dr\right. \\ &\left. -\tfrac{1}{2}(\varepsilon_{1s}+\varepsilon_{ns}+F^0_{ns})\int_0^{\infty} P_{ns}F_{ks}\,dr\right).\end{aligned} \tag{2.14}$$

A_a may also be evaluated by extrapolating the excitation partial collision strengths Ω_c and using correspondence principle arguments (see Burgess 1965a, 1966). We may then identify Ω^I_b (of 2.5) with $(2\zeta^2/\pi\nu^3)\Omega^I_c$, where $\nu = n - \mu$ is the effective principal quantum number of the *nl* state and $\zeta = Z - 2$. However, in the collision problem we also have the unitarised collision strength Ω^{II}_c which satisfies conservation of flux and also allows (to a certain extent) for coupling to neighbouring states and so could be expected to lead to a more complete description of the autoionisation process than Ω^I_c or equivalently the A_a given by (2.5). Thus, the correction factors that we use for A_a are those obtained from the (extrapolated) ratios of the five-state unitarised CEDW2 or CEDW3 partial collision strengths to those of the non-unitarised Coulomb-Bethe approximation.

2.3. Radiative transition rates

The dipole radiative transition probability rate A_r is given by (see, for example, Cowan 1981)

$$A_r(t' \to t) = \frac{64\pi^4 e^2 a_0^2}{3h\lambda^3}\frac{\mathcal{S}(t, t')}{\omega(t')} \tag{2.15}$$

$$= 2.6775 \times 10^9\,(\Delta E)^3 \frac{\mathcal{S}(t, t')}{\omega(t')}\,s^{-1} \tag{2.16}$$

where the emitted photon has a wavelength λ and an energy ΔE (Rydbergs). The states $t' = C'SL'p'$ and $t = CSLp$ are of opposite parity and have $|L - L'| \leq 1$. The line strength $\mathcal{S}$ may be written in terms of the dipole operator $\boldsymbol{P}^{(1)}$ as follows

$$\mathcal{S}(t, t') = \sum_{\substack{M_S M_{S'} \\ M_L M_{L'}}} |\langle tM_S M_L|\boldsymbol{P}^{(1)}|t'M_{S'}M_{L'}\rangle|^2 \tag{2.17}$$

where

$$\boldsymbol{P}^{(1)} = \sum_{n=1}^{3} \boldsymbol{r}_n. \tag{2.18}$$

Using equation (5.4.1) of Edmonds (1957), $\mathcal{S}$ may be written in terms of a reduced matrix element; thus

$$\mathcal{S}(t, t') = (2S+1)\delta_{SS'}|\langle t\|\boldsymbol{P}^{(1)}\|t'\rangle|^2. \tag{2.19}$$

For Li-like ions we consider (for $nl \neq n_c l_c$)

(*a*) $$1sn_c p(^w P)nl^{*\,2}L' \rightarrow 1s^2(^1S)nl\,^2L + h\nu_a$$

and

(*b*) $$1sn_c l_c(^w L_c)np\,^2L' \rightarrow 1s^2(^1S)n_c l_c\,^2L_c + h\nu_b.$$

Again using the equivalent-electron frozen-core approximation and the three-electron wavefunction of III, we obtain for $\langle t\|\boldsymbol{P}^{(1)}\|t'\rangle$

(*a*) $\langle 1s^2(^1S)nl\,^2L\|\boldsymbol{P}^{(1)}\|1sn_c p(^w P)nl^{*\,2}L'\rangle$

$$= {}^wN^{-1/2}\langle l0L\|c^{(1)}\|l1L'\rangle\left(b_w\int_0^\infty F_{nl}F^*_{nl}\,dr\int_0^\infty P_{n_c p}rP_{1s}\,dr\right.$$
$$\left.+\,\delta_{l1}h_w\int_0^\infty P_{n_c p}F_{np}\,dr\int_0^\infty F^*_{np}rP_{1s}\,dr\right) \tag{2.20}$$

and

(*b*) $\langle 1s^2(^1S)n_c l_c{}^2L_c\|\boldsymbol{P}^{(1)}\|1sn_c l_c(^w L_c)np^2L'\rangle$

$$= {}^wN^{-1/2}\langle l_c0L_c\|\boldsymbol{c}^{(1)}\|l_c1L'\rangle$$
$$\times\left(b_w\delta_{l_c1}\int_0^\infty F_{n_c p}F_{np}\,dr\int_0^\infty P_{n_c p}rP_{1s}\,dr\right.$$
$$\left.+\,h_w\int_0^\infty F_{np}rP_{1s}\,dr\int_0^\infty P_{n_c l_c}F_{n_c l_c}\,dr\right). \tag{2.21}$$

For equivalent electrons ($nl = n_c p$) we consider

$$1s(^2S)np^2(^wL')^2L' \rightarrow 1s^2(^1S)np\,^2P + h\nu$$

where ${}^wL' = {}^1S$, ${}^1D$ or ${}^3P$. However, the ${}^3P$ case cannot autoionise to $1s^2kl$. $\langle t\|\boldsymbol{P}^{(1)}\|t'\rangle$ is then given by

$\langle 1s^2(^1S)np\,^2P\|\boldsymbol{P}^{(1)}\|1s(^2S)np^2(^wL')^2L'\rangle$

$$= 2^{1/2}\langle 101\|\boldsymbol{c}^{(1)}\|11L'\rangle h_w\int_0^\infty P_{np}F_{np}\,dr\int_0^\infty P_{np}\,rP_{1s}\,dr. \tag{2.22}$$

Using equation (7.1.8) of Edmonds (1957) we obtain

$\langle ll'_c L'\|\boldsymbol{c}^{(k)}\|l_c L\rangle$

$$= (-1)^{l+l_c+L'+k}[(2L+1)(2L'+1)]^{1/2}\begin{Bmatrix} l'_c & L' & l \\ L & l_c & k\end{Bmatrix}\langle l'_c\|\boldsymbol{c}^{(k)}\|l_c\rangle \tag{2.23}$$

and using equation (5.4.6) of Edmonds (1957) we have that

$$\langle l'_c\|\boldsymbol{c}^{(k)}\|l_c\rangle = (-1)^{l'_c}[(2l'_c+1)(2l_c+1)]^{1/2}\begin{pmatrix} l'_c & \mathrm{k} & l_c \\ 0 & 0 & 0\end{pmatrix}. \tag{2.24}$$

Then for $k = 1$ and $l'_c = l_c \pm 1$

$$\langle l'_c\|\boldsymbol{c}^{(1)}\|l_c\rangle = \pm l_>^{1/2} \tag{2.25}$$

where $l_> = \max(l_c, l'_c)$. Expressions for the square of (2.23) have been given by Burgess and Seaton (1960) who also tabulate the most likely cases. However, for s-p transitions

(2.23) is readily simplified to give

$$|\langle ll'_c L' \| \boldsymbol{c}^{(1)} \| ll_c L \rangle|^2 = \tfrac{1}{3}(2L''+1) \tag{2.26}$$

where

$$L'' = l \pm 1 = \begin{cases} L' & \text{for p} \to \text{s, i.e. } l'_c = 1 \\ L & \text{for s} \to \text{p, i.e. } l_c = 1. \end{cases}$$

3. Results for Fe^{24+}

We define $F(n_c, n)$ by

$$F(n_c, n) = \sum_{\substack{ll_c \\ wL}} \frac{\omega(j, nl)}{\omega(i)} b(j, nl) \Big(A_r(j, nl \to i, nl) + A_r(j(n_c l_c), nl \to i, n_c l_c) \Big) \tag{3.1}$$

where $i = 1s^2\ {}^1S$ and $j, nl = 1s n_c l_c ({}^w L_c) nl\ {}^2L$. This is a useful quantity for comparison of results since it depends only on n_c and n and we expect these to be good quantum numbers, provided that there is little mixing between configurations belonging to different complexes. We note that if the energy factor in the exponential in $\alpha_d(i; \text{tot})$ (see equations (2.1) and (2.3)) were independent of the resonances then $\Sigma_{n,n_c} F(n_c, n)$ would be directly proportional to $\alpha_d(i; \text{tot})$.

We have calculated $F(n_c, n)$ directly for $2 \leqslant n_c \leqslant n \leqslant 5$ in LS coupling with no configuration mixing, using both the CEDW1 and CEDW3 radial equations for the (nl) spectator electron. The nuclear charge dominates the structure of the radial functions for Fe^{24+} and the inclusion of exchange-distorting potentials (CEDW3) gives results for $F(n_c, n)$ that differ by less than 1% from those presented in tables 1 and 2, which were calculated with non-exchange radial functions (CEDW1). Parentage is not a good quantum number for intermediate states of the form $1snl({}^wS)np$ and so we have also calculated A_a and A_r allowing for parental mixing, using the mixing coefficients of SUPERSTRUCTURE (see Eissner *et al* 1974), care being taken to ensure phase consistency.

In table 1 we compare our results for $F(2, n)$ with those that we have derived from the configuration-mixing intermediate-coupling results of Bely-Dubau *et al* (1979a tables 2 and 3, 1979b table 1). Bely-Dubau *et al* (1979b § 4) state that the lowest terms missing from their estimate of the total di-electronic recombination rate coefficient are of the form $1s3l3l'$. However, their graph (Bely-Dubau *et al* 1979b figure 6) is consistent

Table 1. Results for $F(2, n)$ in units of s^{-1}.

		n			
		2	3	4	5
This paper	No mixing	1.5624 (15)†	9.567 (14)	4.209 (14)	2.194 (14)
	Parental mixing	1.328 (15)			
Derived from Bely-Dubau *et al* (1979a, b)		1.368 (15)	9.99 (14)	4.24 (14)	

† 1.5624 (15) means 1.5624×10^{15}.

with their results for $F_2(n)$ (table 2 of Bely-Dubau *et al* 1979b p 808) which are for satellites to the $n_c = 2$ resonance line, which corresponds to the first A_r term in (3.1). They do not include the contribution from $n_c = 2$ satellites to the $n = 3, 4$, etc resonance lines (which arise from intermediate states of the form $1s2l3l'$, $1s2l4l'$, etc) which corresponds to the second A_r term in (3.1). This is clear from summing the individual line factors in table 3 of Bely-Dubau *et al* (1979a p 410) and table 1 of Bely-Dubau *et al* (1979b p 804) and comparing them with the values of $F_2(3)$ and $F_2(4)$ given in table 2 of Bely-Dubau *et al* (1979b p808). In other words, while they include $n \to 1$ core stabilisations in the branching ratio $[A_a/(A_a + \Sigma A_r)]$ they do not include them in the numerator of $F_2(n)$ for $n \geqslant 3$; their $F_2(2)$ is of course directly comparable with our $F(2, 2)$. For $n = 3$ and 4 we have added to their value for $F_2(n)$ the contribution from the $n_c = 2$ satellites to the $n = 3$ and 4 resonance lines, using their results for ΣA_r, to obtain a value comparable with $F(n_c, n)$, assuming that ΣA_r is dominated by $n \to 1$ transitions. There still remains of course the contribution from the $n_c = 2$ satellites to the $n > 4$ resonance lines.

The reason that a significant contribution to $F(2, n)$, for $n > 2$, arises from allowing the spectator electron to radiate lies mainly in the spin coupling. The 2p core electron radiation via the singlet parent channels dominates that due to the np spectator electron. The same is not true for the triplet parent channel which is almost forbidden to the 2p electron but not the np. However, both parent terms are free to auto-ionise (see equation (2.7)). Of course, in the case of the 2s core electron, the radiation due to the np spectator electron dominates both parental channels.

We note that if $A_a \ll A_r$ then $\alpha_a(i; \text{tot}) \simeq \text{constant} \times \Sigma \omega A_a$ and that if we make a unitary transformation $U: A_a \to \bar{A}_a$ (and $A_r \to \bar{A}_r$) such that $\bar{A}_a \ll \bar{A}_r$ then $\bar{\alpha}_d(i; \text{tot}) \simeq \text{constant} \times \bar{\Sigma} \bar{\omega} \bar{A}_a$. Since U is unitary $\Sigma \omega A_a = \bar{\Sigma} \bar{\omega} \bar{A}_a$ and it follows that $\alpha_d \simeq \bar{\alpha}_d$. This is the underlying reason for the close agreement in table 1 between our results and those of Bely-Dubau *et al* (1979a, b). Of course $\exists$ cases such that $A_r = 0$, $A_a \neq 0$ with $\bar{A}_r \neq 0$ (and $A_a \neq 0$), our results imply that these are unimportant. $A_a \leqslant A_r$ for the $1s2l2p$ configurations and so parental mixing (for $l = 0$) is important for $F(2, 2)$. However, $A_a \ll A_r$ for $1snlnp$ $(n > 2)$ and although parental mixing is still strong for $l \neq 1$ it has little affect on $F(n, n)$ as can be seen from table 2 where we present our results for $F(n_c, n)$ for $3 \leqslant n_c \leqslant n \leqslant 5$.

To get the contribution to $\alpha_d(i; \text{tot})$ from $n > 5$, $n_c \geqslant 2$ we evaluate $F(n_c, n)$ by extrapolation. We can extrapolate $F(2, n)$ upwards using the n^{-3} asymptotic dependence of A_a; $F(2, 5)$ extrapolated thus from $F(2, 4)$ differs by 2% from the value

Table 2. Results for $F(n_c, n)$ in units of s^{-1}.

		n		
n_c		3	4	5
3	No mixing	1.596 (14)	1.210 (14)	6.121 (13)
	Parental mixing	1.507 (14)		
4	No mixing		2.788 (13)	2.583 (13)
	Parental mixing		2.722 (13)	
5	No mixing			7.173 (12)

calculated directly. We can also extrapolate downwards the collision results of IV, as described in § 2, to obtain the contribution to $F(2, n)$ from the singlet parents. The extrapolated result for $F(2, 4)$ differs by less than 2% from that of the direct calculation and this is a maximum bound on the error of $F(2, n)$ for $n \geqslant 4$. For this reason we use the downward extrapolation results for the singlet parents of $F(2, n)$ for $n > 5$ and extrapolate upwards still for the triplet parents. We could extrapolate downwards to get $F(n_c, n)$ for $n > 5$, $n_c \geqslant 3$ using the same ratios of collision strengths as for $F(2, n)$. However, the extrapolated value for $F(3, 5)$ differs by about 20% from the value calculated directly, while the value extrapolated upwards from $F(3, 4)$ differs by only 1%. Thus we extrapolate upwards to evaluate $F(n_c, n)$ for $n > 5$, $n_c \geqslant 3$.

We present our results for $\alpha_d(i; \text{tot})$ for Fe^{24+} in figure 1. We have used our parental mixing results where available and also allow for the full $n_c l_c nl$ dependence of E for $2 \leqslant n_c \leqslant n \leqslant 5$ while for $n > 5$, $n_c \geqslant 2$ we take E to be dependent only on n_c and n. We find that di-electronic recombination via intermediate states of the form $1s2l_c nl$ (i.e. a $1 \rightarrow 2$ core excitation) contributes 90% of the total rate and that via $1s3l_c nl$ ($n \geqslant 3$) contributes 7%. Table 1 indicates that the results of our calculation for $\alpha_d(i; \text{tot})$ would be accurate to approximately 5% when compared with a full multiconfiguration intermediate-coupling calculation. We have also reproduced the curve of Bely-Dubau *et al* (1979b) in figure 1 and we see that their results, which are only for satellites to the $n_c = 2$ resonance line and not for the $1 \rightarrow 2$ core excitation as stated in their paper, represent only 77% of the total di-electronic recombination rate coefficient and not 90% as they claimed (Bely-Dubau *et al* 1979b); at $T = 4 \times 10^7$ K $- \alpha_d^{BD} = 4.80 \times 10^{-13}$ cm^3 s^{-1} compared with $\alpha_d^{NRB} = 6.20 \times 10^{-13}$ cm^3 s^{-1}. The good agreement at low temperatures between our results and those of Bely-Dubau *et al* (1979b) arises because of the presence of the exponential factor in (2.1) which causes $\alpha_d(i; \text{tot})$ to be dominated by the contribution from the $n = 2$ satellites to the $n_c = 2$ resonance line. The results of Nasser and Hahn (1983) (not shown) which include contributions from states of configurations of the form $1s2l_c nl$ and $1s3l_c 3l$, agree to about 10% with our results and indicate that their simplified procedure is quite reliable here.

The results of the general formula of Burgess (1965b) are also shown in figure 1 and they lie 33% above our results at $T = 4 \times 10^7$ K ($\alpha_d^{GF} = 8.21 \times 10^{-13}$ cm^3 s^{-1}). We

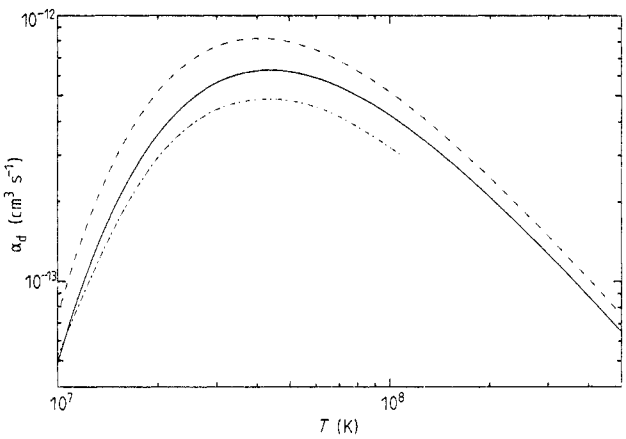

Figure 1. Di-electronic recombination rate coefficients for Fe^{24+}. ——, total (this paper); - - -, total (GF Burgess 1965b); - · - · -, from sum of satellites to the $n_c = 2$ resonance line (Bely-Dubau *et al* 1979b).

note that the results of the Burgess GF for the $2 \rightarrow 1$ core stabilisation are incorrectly represented in the paper by Bely-Dubau *et al* (1979b, see Bely-Dubau *et al* 1983). The formula of Merts *et al* (1976), which is a modification of the Burgess GF for $\Delta n_c \neq 0$, gives poor results (not shown, see Bely-Dubau *et al* 1983 figure 2). The Merts formula is based in part on the results of Shore (1969), which have been shown to be in error by Burgess and Tworkowski (1976) and so the validity must be questioned.

Bitter *et al*(1979, 1981) have observed the $n = 2$ and 3 satellites to the $n_c = 2$ resonance line and they are in good agreement with the results of Bely-Dubau *et al* (1979a, b, see Bely-Dubau *et al* 1983). However, these experimental results (not shown) only contribute about 50% towards the total di-electronic recombination rate.

4. Conclusion

We have shown that, due to the high nuclear charge, very accurate results (5%) for the total di-electronic recombination rate coefficient of Fe^{24+} can be obtained from a single-configuration *LS*-coupling calculation (supplemented by parental mixing of the 1s2s2p configuration). As Z decreases we no longer have $A_a \ll A_r$; thus the neglect of configuration mixing and intermediate coupling will have to be re-assessed as will the neglect of autoionisation into the continuum of excited configurations. The first two effects redistribute the existing flux (for A_a and A_r separately) between the intermediate states rather than generate new flux. Thus, on summing over all intermediate states, the differences in estimates of $\alpha_d(i; \text{tot})$ arise from differences in the competition between A_a and A_r and the need for configuration mixing and intermediate coupling will depend on how systematic these differences are. Distortion effects also become more important in the evaluation of the radial functions as Z decreases and so we need to pursue the use of exchange-distorted wavefunctions both in simple calculations of the type considered here and as the input to configuration-mixing and intermediate-coupling calculations.

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References

Badnell N R 1983a *J. Phys. B: At. Mol. Phys.* **16** 3263-78

—— 1983b *Cambridge Department of Applied Mathematics and Theoretical Physics Report DAMTP/AA/-1000-NRB*

—— 1984 *J. Phys. B: At. Mol. Phys.* **17** 4013-32

—— 1985 *J. Phys. B: At. Mol. Phys.* **18** 955-66

Bell R H and Seaton M J 1985 *J. Phys. B: At. Mol. Phys.* **18** 1589-629

Bely-Dubau F, Bitter M, Dubau J, Faucher P, Gabriel A H, Hill K W, von Goeler S, Sauthoff N and Volonté S 1983 *Phys. Lett.* **93A** 189-92

Bely-Dubau F, Dubau J, Faucher P, Gabriel A H, Loulergue M, Steenman-Clark L, Volonté S, Antonucci E and Rapley C G 1982a *Mon. Not. R. Astron. Soc.* **201** 1155-69

Bely-Dubau F, Dubau J, Faucher P and Steenman-Clark L 1981 *J. Phys. B: At. Mol. Phys.* **14** 3313-24

Bely-Dubau F, Faucher P, Steenman-Clark L, Bitter M, von Goeler S, Hill K W, Camhy-Val C and Dubau J 1982b *Phys. Rev.* A **26** 3459-69
Bely-Dubau F, Gabriel A H and Volonté S 1979a *Mon. Not. R. Astron. Soc.* **186** 405-19
—— 1979b *Mon. Not. R. Astron. Soc.* **189** 801-16
Bhalla C P, Gabriel A H and Presnyakov L P 1975 *Mon. Not. R. Astron. Soc.* **172** 359-75
Bitter M, von Goeler S, Hill K W, Horton R, Johnson D, Roney W, Sauthoff N, Silver E and Stodiek W 1981 *Phys. Rev. Lett.* **47** 921-3
Bitter M, Hill K W, Sauthoff N R, Efthimion P C, Meservey E, Roney W, von Goeler S, Horton R, Goldman M and Stodiek W 1979 *Phys. Rev. Lett.* **43** 129-32
Boiko V A, Pikuz S A, Safronova U I and Faenov A Ya 1978 *Mon. Not. R. Astron. Soc.* **185** 789-805
Burgess A 1964 *Astrophys. J.* **139** 776-80
—— 1965a *Ann. Astrophys.* **28** 774-8
—— 1965b *Astrophys. J.* **141** 1588-90
—— 1966 *Auto-ionization* ed A Temkin (Baltimore: Mono) pp 25-31
Burgess A and Seaton M J 1960 *Mon. Not. R. Astron. Soc.* **120** 121-51
—— 1964 *Mon. Not. R. Astron. Soc.* **127** 355-8
Burgess A and Tworkowski A S 1976 *Astrophys J.* **205** L105-7
Chichkov B N, Mazing M A, Shevelko A P and Urnov A M 1981 *Phys. Lett.* **83A** 401-3
Cowan R D 1981 *The Theory of Atomic Structure and Spectra* (Berkeley: University of California Press)
Davies P C W and Seaton M J 1969 *J. Phys. B: At. Mol. Phys.* **2** 757-65
Dubau J and Volonté S 1980 *Rep. Prog. Phys.* **43** 199-251
Edlén B and Tyrén F 1939 *Nature* **143** 940-1
Edmonds A R 1957 *Angular Momentum in Quantum Mechanics* (Princeton: Princeton University Press)
Eissner W, Jones M and Nussbaumer H 1974 *Comput. Phys. Commun.* **8** 270-306
Fuhr J R, Martin G A, Wiese W L and Younger S M 1981 *J. Phys. Chem. Ref. Data* **10** 305-565
Gabriel A H 1972 *Mon. Not. R. Astron. Soc.* **160** 99-119
Gabriel A H and Jordan C 1969 *Nature* **221** 947-9
—— 1972 *Case Studies in Atomic Collision Physics* vol 2, ed M R C McDowell and E W McDaniel (Amsterdam: North-Holland) pp 209-91
Gabriel A H and Paget T M 1972 *J. Phys. B: At. Mol. Phys.* **5** 673-85
Massey H S W and Bates D R 1942-3 *Rep. Prog. Phys.* **9** 62-74
Merts A L, Cowan R D and Magee N H 1976 *Los Alamos Scientific Laboratory: Informal Report LA-6220-MS*
Nasser I and Hahn Y 1983 *J. Quant. Spectrosc. Radiat. Transfer* **29** 1-9
Seaton M J 1983 *Rep. Prog. Phys.* **46** 167-257
Seaton M J and Storey P J 1976 *Atomic Processes and Applications* ed P G Burke and B L Moiseiwitsch (Amsterdam: North-Holland) pp 133-97
Shore B W 1969 *Astrophys. J.* **158** 1205-18
Steenman-Clark L, Bely-Dubau F and Faucher P 1980 *Mon. Not. R. Astron. Soc.* **191** 951-9