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FOREWORD

This report is based on remarks made by the author to the Workshop on Problems and Prospects in Electron-Positive, Ion Physics held at the Joint Institute for Laboratory Astrophysics, University of Colorado, July 1 and 2, 1974.

CALCULATIONAL ASPECTS OF COLLISIONAL EXCITATION OF IONS IN HOT SOLAR PLASMAS

I. ASTROPHYSICAL APPLICATION

The first purpose of these remarks is to bring to the attention of the atomic scattering community the cross section requirements of physicists studying UV and X-ray emission spectra associated with active and flare-produced plasmas in the sun's corona. The studies that are of specific concern here are an integral part of an experimental satellite program (OSO-5, OSO-7) of the Goddard Space Flight Center group (Neupert et al.[1]), and in the final section of this report we shall give specific categories of excitations corresponding to prominent coronal lines which they observe under solar disturbed conditions.

In this first section I shall outline briefly the astrophysical background leading to the kind of atomic cross section needed and to discuss the shortcomings of presently available methods and programs. The second section deals with our general approach (the distorted wave approximation) to the calculational problem. The third section will consist of two parts: one discusses the effect of resonances in a very qualitative way and gives a few words on how their effect is included through the multichannel quantum defect theory. In the second part we derive the threshold law for electron-atomic hydrogen excitation in the distorted wave approximation. The fact that the approximation is able to reproduce that very non-trivial result is as convincing an argument as we can adduce of the power of the method.

The presence of extremely hot material in the sun's corona is indicated among other things by the omission of EUV and X-ray lines. We are here concerned with the coronal counterparts of active centers [$T_e \simeq (3\text{-}4) \times 10^6$ °K, $N_e \simeq 10^9 - 10^{10}$ cm^{-3}] and flare produced plasmas [$T_e \simeq (10\text{-}40) \times 10^6$ °K, $N_e \simeq 10^{10} - 10^{11}$ cm^{-3}]. In all coronal plasmas there is a balance between ionization by electron impact and recombination by radiative and dielectronic processes. Transitions from ions with closed shells feature prominently (cf. Fig. 2, p. 12).

Most X-ray and UV line emission occurs as a result of electron collisions. The analysis of these spectra is usually done in terms of an energy average rate coefficient

$$C_{ij}(T) = \int f_T(v)\, v\, Q_{ij}(v)\, dv \, \frac{cm^3}{sec} , \qquad (1.1)$$

where $f_T(v)$ is a Maxwellian electron distribution of velocities v corresponding to a temperature T. The ultimate atomic parameter needed is seen to be in the cross section Q_{ij} .

It is the evaluation of Q_{ij} (i = initial state, j = final state) then that is the chief concern of the atomic calculation. We sketch in a few words what has obviously been a long story. Van Regermorter[2] has given a formula and coefficients, based on the Bethe approximation, for optically allowed transitions. The Coulomb-Born approximation has been applied by Burgess, Hummer, and Tully[3] and by Blaha[4] for a variety of cases. As invaluable as these and many other calculations are, we believe they are not really sufficiently accurate for the needs of the solar disturbed problem for the following reasons:

(i) Even though the temperature is high, the mean energy of the electrons is generally lower than that of the orbital electrons of the highly stripped ions of relevance here. Thus a basic criterion for the validity of the Coulomb-Born approximation is not fulfilled.

(ii) For the same reason the consistent (by which I mean an approximation better than Born-Oppenheimer) inclusion of the exchange symmetry between the scattered and orbital electrons is necessary.

(iii) Because of the considerable excess of nuclear charge over number of electrons, a great number of autoionization states (i.e. resonances), of the electron-ion system in the inelastic domain start playing an important role. This is one aspect of a non-trivial quantum mechanical phenomenon which shows up in electron-neutral scattering at energies closer to impact ionization threshold. We shall discuss this more below, but suffice it to say now that the high charge of the nucleus enables this phenomenon to be included effectively, analytically,[6] and it is our hope to be able to include these important developments in the Goddard program.

II. THE DISTORTED WAVE APPROXIMATION

In the form that we shall be concerned with it here, the distorted wave approximations starts from two equivalent exact expressions for the excitation cross section.

$$Q_{if} = \frac{k_f}{k_i} |\langle \Phi_f | V_f | \Psi_i^{(+)} \rangle|^2 = \frac{k_f}{k_i} |\langle \psi_f^{(-)} | V_i | \Psi_i \rangle|^2 \qquad (2.1)$$

$\Psi_{i,f}^{(\pm)}$ are exact wave functions corresponding to initial conditions with outgoing radial wave scattering (upper sign) parts or final state solutions with ingoing radial (lower signs) waves. k_i and k_f are the initial and final momenta. $\Phi_{i,j}$ are wave functions corresponding to unperturbed initial (final) states, i.e. they are solutions of the Schrödinger equation with V_f (V_i) absent from the Hamiltonian.

The distorted wave approximation, as we shall use it, consists of replacing the exact solution by an approximate solution which is a one channel function corresponding to elastic scattering from the initial or final state at the appropriate energy. As work of Shelton et al.[7] and McDowell et al.[8] has shown, this is an excellent approximation for inelastic scattering of electrons from neutral atoms. By writing down this form of the distorted wave (assuming here that the target state has zero angular momentum).

$$\Psi \to \Psi_{DW} = \mathcal{A}\left\{\sum_{\ell} \frac{u_\ell(r_1)}{r_1} Y_{\ell 0}(\Omega_1)\, \Phi_{target}(2, \ldots, N+1)\right\}. \qquad (2.2)$$

one can see that since the distorted wave function is antisymmetrized ($\mathcal{A}$) thus the effects of exchange have dynamical meaning in that they will give additional terms in the equation determining $u_\ell(r)$. Secondly, since a sum over partial waves is involved, there is no assumption of high energy. (In fact the lower the energy the better since fewer partial waves need be included until convergence is achieved). In addition to these well-known advantages of the distorted wave method there are additional circumstances which benefit the highly ionized charged target application. Because the attraction to the nucleus so outweights the mutual repulsion between the orbital electrons, a very simple approximation of the target wave function, Φ_{target}, suffices. (It should be realized that an approximation is always required for any many-electron target.) For the same reason the polarization of the target by the incoming electron, which can be very important for neutral targets,[9] is negligible here. There is an implicit restriction that Z not be so large that relativistic effects become dominant; however various calculations[10] indicate that relativistic effects are not too important for $Z < 26$ (which is the case of iron, almost the highest Z of direct concern in this astrophysical application - cf section IV).

Ideally the functions $u_\ell(r_1)$ would be numerical solutions of the exchange approximation equation obtained by substituting (2.2) into a variational principle for the scattering phase shift. The general programs however that have so far been written[6] use a scaled Thomas-Fermi potential with an orthogonality constraint to simulate exchange.[6,11] The approximation seems adequate although somewhat less than what one might optimally desire. However we shall not pursue that aspect of the matter any further in this report.

III. OTHER ITEMS

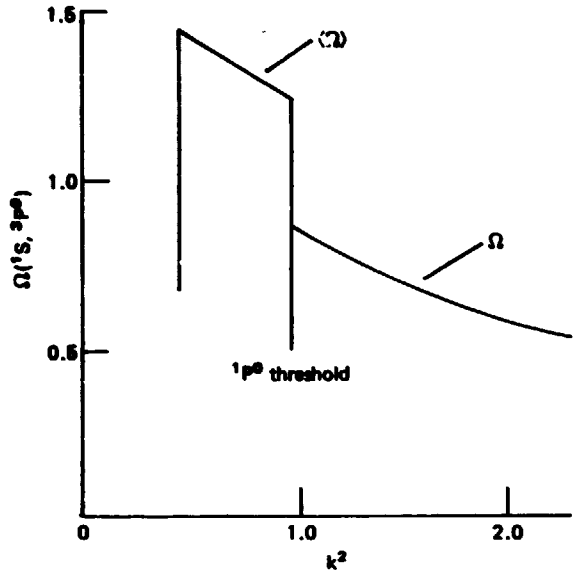
In this section I shall discuss two items which are relevant to the present problems and approach. The first has to do with the incorporation of resonances, whose effect is a major one in these applications; the second derives an analytical form of a threshold law in the distorted wave approximation which we have not previously seen, and thereby gives further evidence of the cogency of the method.

It is by now well known that in the scattering of electrons from atoms resonance can occur.[12] The major class of these resonances occurs just below the energies of the various excited state of the target atom. Although the neutron counterparts of these resonances are a classic feature of nuclear physics, it is only within the last 12 years that they have had their most natural and mathematical explanation in the work of Feshbach[13] in a way which if anything is even more suitable to the atomic problem; they are accordingly and appropriately called Feshbach resonances. Qualitatively they can be described as states of the electron plus target system which are only weakly coupled to energetically allowable open channels. Since the easiest way of forming these states is by attaching the incoming electron to an excited state of the target system (which by definition means the target has one its electrons in an excited orbital), they are sometimes called doubly excited states, (this picture also explains why the resonant energies are generally just below the excited state energies of the target).

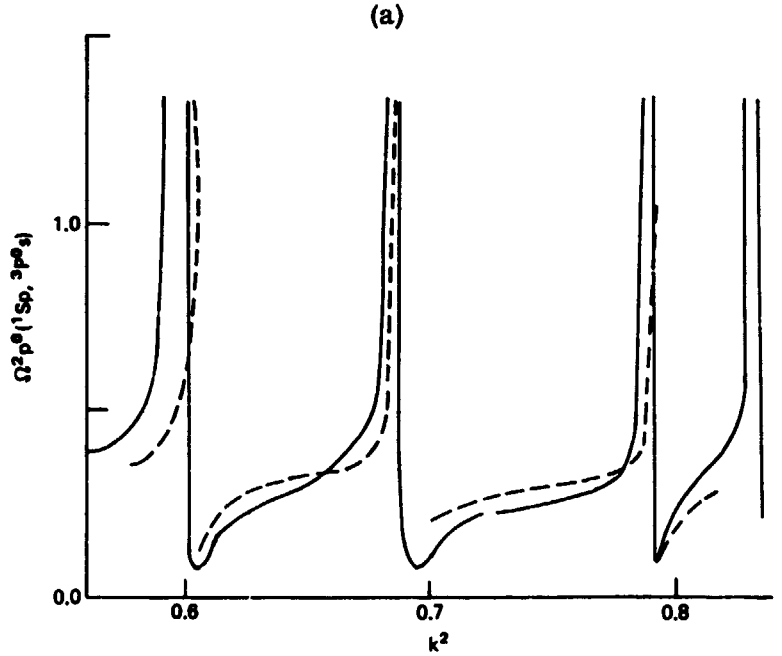
Now exactly the same phenomenon can occur in electron-ion scattering except that as the charge of the nucleus increases relative to the number of electrons, the energies of these autoionization states descend ever farther below the parent excited state until they finally descend below even lower excited states of the target ion. Thus if one is dealing with a highly stripped ion in the region, say between the first and second excited states, there will be many classes of resonances which will span the whole energy region and they can have an important average effect. This is well demonstrated in a calculation of Hershkowitz and Seaton[6] reproduced in Figure 1 wherein the average of the collision strength,

$$\Omega_{ij} = k_i^2 (2S_i + 1)\,(2L_i + 1)\,Q_{ij}, \tag{3.1}$$

for e - CIII excitation is seen to be augmented by 50% when states attached to the P° threshold are included. (I do not believe that the calculation is intended to imply that the cross section drops sharply at that threshold. Presumably resonances attached to even more excited states would take over.) The effect of such resonances can be expected to be even larger for more highly charged targets.



(a)



(b)

Figure 1. (a) The enhancement of the average collision strength in e-CIII excitation due to resonances whose parent state is 1p°. (b) The individual resonances from the partial waves corresponding to incoming p wave and outgoing s wave of the impacting electron. Dashed curves are distorted wave results and solid curves are the full close coupling results. Both figures from Hershkowitz and Seaton, Ref. 6.

Fortunately this effect can be included within the distorted wave formalism. The point is that the scattering is dominated by the known (Coulomb) solutions of the electron from the ionic core. The many-body effects of the core electrons can be incorporated in terms of quantum defects below threshold which can be analytically continued into Coulomb phase shifts above threshold. One can partition the scattering matrix into open and closed channels and, using this connection, obtain from open channel distorted wave calculations, the closed channel (resonant) effect on other channels which are open.

The analytic and programmatic aspects of these problem have been the subject of much work and development particularly at University College, London as exemplified in Refs. 6, 11 and 14. (We are most grateful to Prof. Seaton and his colleagues in advance for the opportunity of availing ourselves of these programs. The work in question will be done in collaboration with Dr. A. K. Bhatia of our group.)

I conclude this section with a brief derivation of the threshold law for excitation of the degenerate (N; ℓ = 0, 1. . N-1) level from the ground state of hydrogen by electron impact. This result, which was first obtained by Gailitis and Damburg[15] in a brilliant but unfortunately not very transparent analysis, is nontrivial not only because the threshold cross section is finite, but because the oscillations away from threshold are (in the complex variable sense) a non-analytic function of the excess energy. The fact then that one can get the correct functional form from the distorted wave approximation speaks for itself about the power of the method. (This analysis also serves as a nice heuristic derivation of this threshold law, which as far as we know has not previously been given.)

We start with a model of the electron hydrogen interaction which was previously introduced in studying the much more difficult impact ionization threshold problem[5]: we replace the electron repulsion r_{12}^{-1} by $(r_1 + r_2)^{-1}$

$$V = -\frac{1}{r_1} + \frac{1}{|r_1 - r_2|} \rightarrow -\frac{1}{r_1} + \frac{1}{r_1 + r_2} \tag{3.2}$$

This corresponds to directions in which the scattered electron (r_1) is opposite to that of the bound electron (r_2), a configuration that dominates the long range interactions, which as we shall show determine the form of the analytical result. Within this model the excitation cross section

$$Q_{iN} = k_N |\langle \Psi_N | V | \Phi_i \rangle|^2 \tag{3.3}$$

corresponds to some kind of an average of the $N\ell$ cross section. The (unperturbed) initial state is the s-wave part of a plane wave on the target in its ground state:

$$\Phi_i = \frac{\sin(k_i r)}{r_1} \frac{R_1(r_2)}{r_2}, \tag{3.4}$$

and the exact final state in the distorted wave approximation is

$$\Psi_N = \frac{F_{k_N}(r_1)}{r_1} \frac{R_N(r_2)}{r_2} \tag{3.5}$$

$R_N(r_2)$ refers to r times the N^{th} hydrogenic s state of the target (R_1 being the ground state). The interaction (3.2a) can conveniently be approximated by[5]

$$V \cong \begin{cases} -\frac{2}{r_1} & (r_1 < r_0) \\ -\frac{b_N}{r_1^2} & (r_1 > r_0) \end{cases} \tag{3.2b}$$

where

$$b_N = 3N^2 \tag{3.6}$$

is the dipole moment of the inner electron and nucleus seen by outer electron.

Substituting (3.5) into usual variational principle (which is equivalent to forming $\int d^3r_2 \frac{R(r_2)}{r_2} (H - E) \Psi_N = 0$), one derives

$$\left(\frac{d^2}{dr^2} - V(r) + k_N^2\right) F_{k_N}(r) = 0 \tag{3.7}$$

With the approximation (3.2b) for V, the exact solution of (3.6) is

$$F_{k_N}(r) = \begin{cases} \eta F_c(k_N r), & r < r_0 \\ F_d(r), & r > r_0 \end{cases} \tag{3.8}$$

F_c is a pure Coulomb move and F_d a linear combination of dipole solutions:

$$F_c = e^{ik_N r} F\left(\frac{1}{k_N} + 1;\ 2;\ 2ik_N r\right) \underset{k_N \to 0}{\to} \sqrt{r}\ J_1(\sqrt{8r}) \tag{3.9a}$$

$$F_d = \sqrt{\frac{\pi}{2k_N}}\, r^{1/2} [J_{i\alpha_N}(k_N r) + BN_{i\alpha_N}(k_N r)]$$

$$\underset{r \to \infty}{\to} \frac{1}{K_N} \sin\left(k_N - \frac{i\alpha_N \pi}{2} - \frac{\pi}{2} + \phi_\alpha\right) \tag{3.9b}$$

J & N are Bessel & Neumann functions and ϕ_α is phase factor depending on B which in turn depends on the matching of function and slope of ηF_c to F_d at $r = r_0$ (i.e. the continuity of the logarithmic derivative $\eta(r_0)$). The normalization constant η is such that it guarantees that inside solution matches to the outside solution, which approaches (the S-wave part of) a plane wave at $r \to \infty$; it is given by[5, 16]

$$\eta = \frac{(r_0 \alpha_N)^{1/2}}{F_c(r_0)\sqrt{k_N}\sqrt{\alpha_N^2 + (r_0 R(r_0) - 1/2)^2}} \tag{3.10}$$

Substituting F_c and its derivative into

$$R(r_0) = \frac{F_c'(r_0)}{F_c(r_0)} \tag{3.11}$$

we find

$$\eta \propto \frac{1}{\sqrt{k_N}} \tag{3.12}$$

Proceeding now very quickly, we find that the inelastic cross section reduces to [we are concerned only with the form thus we set B = 0 in Eq. (3.9b)]

$$Q_{iN} \propto k_N \left| \frac{1}{\sqrt{k_N}} \int_0^{r_0} F_c(r)\, V_{N1}(r) \sin k_i r dr \right.$$

$$\left. + \frac{1}{\sqrt{k_N}} \int_{r_0}^{\infty} r^{1/2} J_{i\alpha_N}(k_N r)\, V_{N1}(r) \sin k_i r dr \right|^2 \tag{3.13}$$

where

$$V_{N1}(r) = \int_0^{\infty} R_N(r_2)\, V(r, r_2)\, R_1(r_2)\, dr_2 \cong \frac{\text{const.}}{[r_0 + 2r]^2} \qquad (\ \cdot$$

is seen to be independent of k_N. And now we let k_N be sufficiently small that

$$k_N r << \alpha_N \Rightarrow k_N << \frac{1}{N}$$

in the region of space which gives the dominant contribution to the integrals. Under these conditions $F_c(r)$ can be replaced by $r^{1/2} J_1(\sqrt{8r})$, a function independent of B_N according to (3.9a), whereas the small argument expansion $J_{i\alpha}(k_N r)$ (of which we only need the real part) is distinctly not independent of k_N:

$$\mathrm{Re}\{r^{1/2} J_{i\alpha}(k_N r)\} \propto r^{1/2} \cos \left[\alpha_N \ln\left(\frac{k_N r}{2}\right) + \phi_\alpha\right] \tag{3.15}$$

Thus from (3.13)

$$Q_{iN} \propto \left| C + \int_{r_0}^{\infty} r^{1/2} \cos \left[\alpha_N \ln\left(\frac{k_N r}{2}\right) + \phi_\alpha\right] \frac{r_0^2 \sin k_i r dr}{(r_0 + 2r)^2} \right|^2 \tag{3.16}$$

The first integral devoted by C is independent of k_N; an asymptotic series can easily be generated for the second integral the leading term of which together with C then provides the final result

$$\lim_{k_N \to 0} Q_{iN} \propto |C_1 + C_2 \cos(\alpha_N \ln k_N + \phi)|^2 \tag{3.14}$$

That is the Gailitis-Damburg[15] result!

IV. ASTROPHYSICAL CROSS SECTION NEEDS

In the context of the astrophysical applications discussed here, i.e. the deduction of temperature and density in solar disturbed regions from the (UV and X-ray) spectral data, the following are relevant transitions for which excitation cross sections are needed. I am indebted to Dr. S. Kastner and to Dr. K. Phillips of Dr. Neupert's group for this information, and especially to Dr. Phillips for astrophysical parts of section I.

Targets

Element	C	O	N	Mg	Al	Si	S	Ar	Ca	Cr	Mn	Fe	Ni
Z	6	8	10	12	13	14	16	18	20	24	25	26	28

Transitions

One-electron

$1s \rightarrow 2s, 2p, 3p, 4p, 5p$

Two-electron

$(1s)^2\ {}^1S \rightarrow (1s\,np)\ {}^1P,\ {}^3P;\ (1s\,n\,s)\ {}^3S$

$n = 2, 3, 4, 5$ ($n > 2$ in order to asses cascade contribution)

Many-electron	wave length region
$(2p)^r \rightarrow (2p)^{r-1}\, n\ell$	15 Å
$(2s)^2\,(2p)^r \rightarrow (2s)\,(2p)^{r+1}$	100 — 200 Å

$r = 1, 2, 3, 4, 5$

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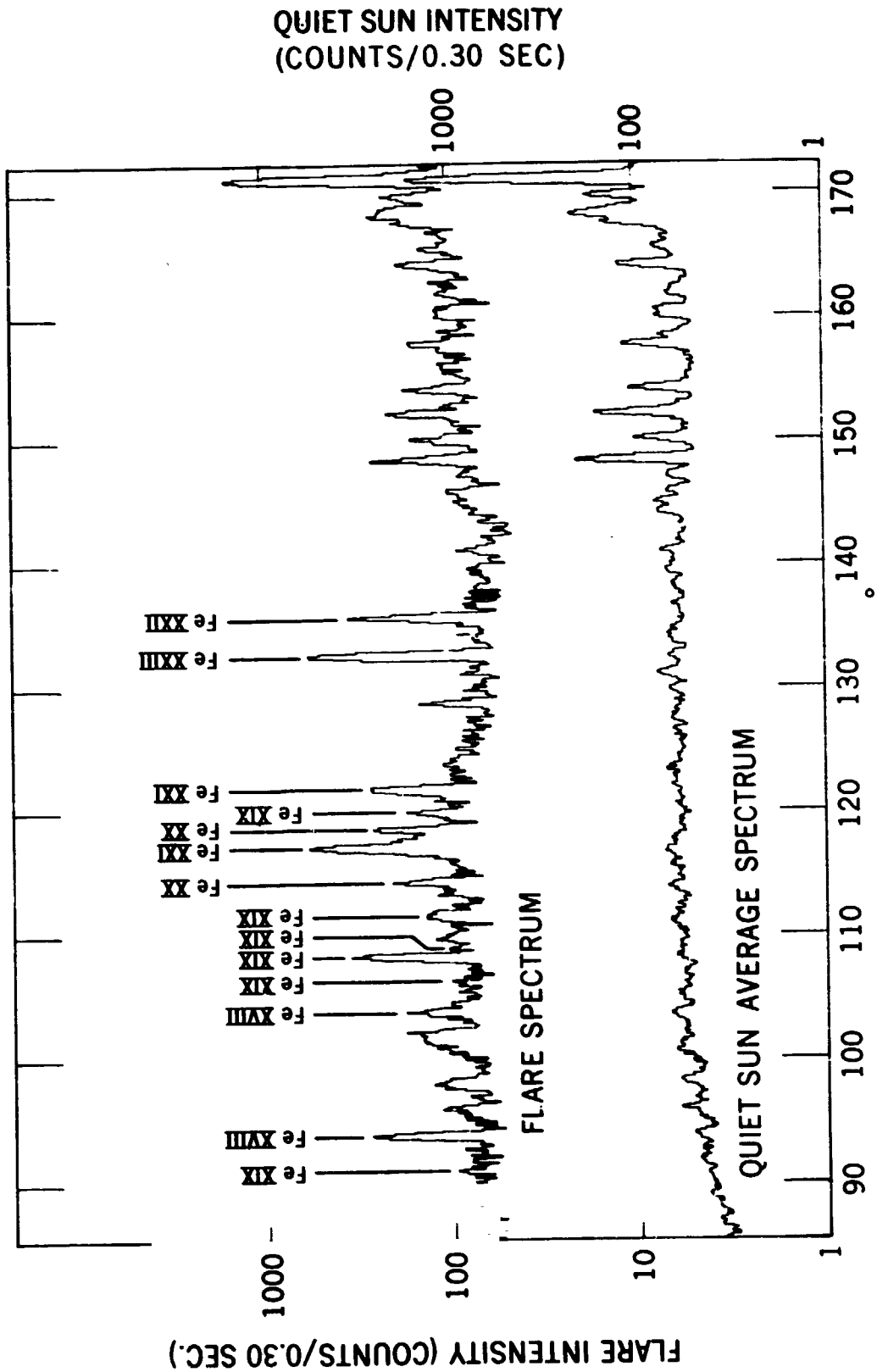

Figure 2: Comparison of flare spectrum (OSO 5) with quiet sun spectrum [from S. Kastner, W. Neupert, M. Swartz Ap. J. 191, 261 (1974)]