ARC DISCHARGE SOURCES

FINAL REPORT
16 OCTOBER 1964 TO 28 FEBRUARY 1967

31 MARCH 1967

CONTRACT Nonr 4647(00)
ARPA ORDER NO. 306-62
CODE 4730
REQ: NO. NR-012-511, 7 ANUARY 1966

A 28-MONTH CONTRACT
EXPIRATION DATE 28 FEBRUARY 1967
COST $195,933

Charles H. Church, Principal Investigator (412) 256-3678

B. W. Swanson	E. Geil
J. Lowke	L. Armstrong
R. Liebermann	G. Basi
P. Buchhave	D. Sun
I. Liberman	R. S. de Voto

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PREFACE

This report presents the work since the previous semiannual report on Contract Nonr 4647(00). It also summarizes the previous work on the contract toward the development of quantitative models for high energy pulsed arcs of the type that are used for the optical pumping of high energy lasers. The studies in this contract have been concerned primarily with xenon as this gas has been used most successfully for high energy laser pumping; the principles contained in the models for the arcs are applicable to other highly radiative arcs, though in many cases the necessary quantitative descriptions of the physical properties of the arc plasma are not available at the present time.

Recent developments in pumping geometries and in additive lamps, arising, in part, from this work and from work in a closely related area, the optical pumping of continuous lasers, under Contracts DA-28-043-AMC-00292(E) and DA-28-043-AMC-02097(E), indicate new promise for efficient optically pumped lasers. The principles discussed in this report provide a basis for an understanding of the optical pumps for lasers.

ABSTRACT

This report summarizes the studies made on Contract Nonr 4647(00) towards the development of models for the highly radiative arcs used for the high energy pumping of lasers. The report also presents the experimental and theoretical studies since the last semi-annual report. The experimental investigations were primarily concerned with more extensive measurements of the spectral radiance of the plasma to provide verification for the models. The theoretical work has resulted in computer methods, described in the appendices, to calculate the transport properties, the spectral absorptivities for the lines and the continuum of xenon, and the spectral radiance and temperature profiles in cylindrical arcs. Also included as an appendix is a theoretical analysis of the xenon arc using radiative transport techniques developed in other studies.

Research Report 67-9C1-ARCSO-R1 May 29, 1967

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I. INTRODUCTION

The optically pumped solid state laser provides the highest peak power and highest peak energy available from coherent sources. This report summarizes the work on Contract Nonr 4647(00) toward the development of quantitative models for the highly radiative arcs used to excite these lasers. Contained in the appendices to this report are computer programs developed in this work for the calculation of many features of these arcs. The calculation procedures are for xenon, though in principle, they are applicable to other atomic systems.

The theoretical and the experimental research on this contract has been directed towards the creation of quantitative models for the flash lamps that in turn would be useful in the improvement of high energy lasers. The development of the models required basic studies of the many aspects of highly radiative arcs, and lead to considerable expansion of the experimental techniques available for the study of these dense plasmas. These plasmas may be encountered in many situations other than the flash tubes for pumping high energy lasers, including re-entry shock waves and high voltage switch gear.

The effort in this contract can be divided into three areas: (1) the development of theoretical techniques to calculate the necessary physical properties of arc plasmas, (2) the applications of these techniques to create models for the high radiative arcs, and (3) the experimental measurements required to formulate and then to verify the models.

The earlier reports (references 1, 2, 3 & 4) described many aspects of the problem more fully. The computer programs resulting from this work are all in the ALGOL language for a Burroughs B5500 DISK computer.

The development of the models required techniques for calculating the transport properties (electrical and thermal conductivity), and the spectral absorptivity (the broadened spectral lines plus the continuum) as a function of temperature and pressure. In addition, methods for handling energy transport within highly radiative inhomogeneous temperature arc plasmas were required.

For the transport properties of xenon, we were fortunate in obtaining the assistance of Dr. R. S. de Voto of Stanford University, who has developed computer programs for calculating the properties of partially ionized monatomic gases. His program for the calculation of the electrical and thermal conductivities of xenon as a function of temperature and pressure is in Appendix A.

The calculation of the spectral absorptivity of xenon required consideration of the broadened lines and the continuum. The final program given in Appendix B is due to the efforts of many people, particularly D. Sun of California Institute of Technology, E. Corinaldesi, now at Boston University, and R. G. Schlecht, now at Aeroneutronics Division of Ford Motor Company. Appendix C uses the bound-bound transition probabilities and other information on xenon to calculate the optical radiation emitted by a cylindrical arc of a given temperature profile and pressure. Appendix D presents calculations for Whittaker functions of real and imaginary argument for use in calculations of the matrix elements for bound-free and free-free transitions. We will discuss details of these calculations in a later section.

Two approaches were followed in the creation of the models for the arc. In one approach, we assumed the arc to be homogeneous in temperature and neglected thermal conduction to the walls. Experimental measurements had indicated that this was a reasonable assumption for the central core. Such model would explain a number of the observed characteristics, such as the arc radiant emission saturation in the infrared and in the visible, and account for a major portion of the input power.

The pressure to be used for this homogeneous temperature model is open to question due to the actual temperature gradient which exists near the walls. In the other approach, the electric field across the arc, the inside diameter of the arc tube, and the pressure of heavy particle number density are to be specified and the radial absolute temperature distribution is to be sought. With the temperature distribution, we could calculate all of the observed properties of the arc including the spectral radiance at the walls (Appendix C). This calculation required the solution to the energy balance equation for a non-gray, nonhomogeneous temperature plasma. An approximate analysis described in Appendix E was applied to this problem to obtain a better initial temperature distribution. The final program developed in this work is given in Appendix F.

The experimental measurements were intended to aid in the formulation and verification of the models. In the course of the work, the flash lamp or more completely, the confined wall-stabilized pulsed arc discharge, was found to be a useful vehicle to study high power density, high pressure, highly radiative plasmas. Plasmas with these characteristics in gases other than xenon are of interest to workers in many fields or research and applications. In the course of this work and in the closely associated company sponsored research, techniques have been and are being developed to study these plasmas. These techniques have included two rapid scanning spectrometers, one of high resolution scanning over a limited range[6] the other of decreased resolution but with a much wider spectral range[7].

A problem still exists in the accurate measurement of the instantaneous pressure. The pressure is crucial to an accurate description of the arc as the pressure varies widely with the temperature gradient near the wall. Currently a laser interferometer similar to that of Gerardo et al.[8] is being set up to allow electron density measurements. These electron density measurements will serve to check the values we have assumed in the calculations.

II. BASIC PRINCIPLES OF HIGHLY RADIATIVE ARCS

The arcs used for pumping high energy lasers have many features in common with arcs used for continuous laser pumping. The primary difference between these arcs lies in the size of the arc column and the power density in the arc. In both cases, the arcs are near or above atmospheric pressure. As the efficiency of the laser systems increase, the differences between the two arc applications are becoming less marked.

The usual form of the arc used in high energy laser pumping is a cylindrical arc surrounded by a wall. We have only investigated this wall stabilized arc. In the arc, current flow carries power into the arc; radiation external to the arc and thermal conduction to the arc surroundings (i.e.: the wall) carry power away from the arc. Convective power transport can be neglected in this type of wall stabilized confined arc unless there is gas flow--which we have not considered in this work. A wall stabilized highly radiative arc such as those used for high energy laser pumping has a central plasma core at the temperature of the fully ionized plasma (the actual temperature varying with the composition of the plasma) with the temperature at the wall dependent upon the rate at which power is carried away from the walls. (A fully ionized plasma may be only .01% ionized. It is characterized by the dominance of the electron-electron and electron-ion interaction over the other particle interaction).

The relation between the input power and that carried away from the arc by radiation and conduction can be put into equation form. Figure 1 presents the family of equations that relate the power input per unit volume to the power carried away by radiation and conduction. We consider the arc to be in local thermal equilibrium (LTE) and thus describable by Boltzmann's equation, Saha's equation and a simple radiation law. The electrical and thermal conductivities as well as the spectral absorptivities are functions of the local temperature and pressure for each constituent. The various constituents of the plasma interact with each other through the ionization law

The Energy Balance

$$\nabla \cdot (\bar{F}_{RAD} + \bar{F}_{TC}) = \sigma\,(p,T)\,E^2$$

where E is the electric field in Volts cm^{-1}, σ is the electrical conductivity in $(ohm\ cm)^{-1}$ and is dependent upon the pressure (p) and the temperature (T). $\bar{F}_{T.C.}$ is the thermally conducted power flux in Watts cm^{-2} and is given by

$$\bar{F}_{T.C.} = -K(p,T)\ \text{grad}\ T$$

K is the thermal conductivity in Watts $cm^{-2}\ {}^{\circ}K^{-1}$ cm. $\bar{F}_{RAD}$ is the radiant emittance (i.e. radiative flux) in Watts cm^{-2} and is expressed in terms of $F_{\nu\,RAD}$, or $F_{\lambda\,RAD}$. The spectral radiant emittance

$$\bar{F}_{RAD} = \int_0^\infty \bar{F}_{\nu\,RAD}\,d\nu = \int_0^\infty \bar{F}_{\lambda\,RAD}\,d\lambda$$

where ν is the frequency and λ the wavelength in consistent units. Consider the x component of $\bar{F}_{\nu\,RAD}$; it is expressed in terms of I_ν:

$$F_{\nu x} = \int_\omega I_\nu(\bar{S})\ \text{Cos}\ (x,\bar{S})\,d\omega$$

I_ν is the spectral radiance (i.e. specific intensity) in Watts cm^{-2} Steradian frequency unit $^{-1}$ along the $\bar{S}$ direction. ω is the solid angle over which the integral is to be taken. I_ν is the solution to the equation of transfer for the geometry being considered:

$$\frac{dI_\nu(\bar{S})}{ds} = \kappa_\nu'(p,T)\,[B_\nu(T) - I_\nu(\bar{S})]$$

in which s is the magnitude of the direction vector $\bar{S}$ and κ_ν' is the spectral absorptivity including stimulated emission in cm^{-1} and is given by

$$\kappa_\nu' = \kappa_\nu(p,T)(1-e^{-h\nu/\kappa T})$$

$B_\nu(T)$ is the Planck distribution function. h is Planck's constant, κ is Boltzmann's constant and are to be in units consistent with T and ν. κ_ν is the spectral absorptivity in cm^{-1} which in turn is the sum of the spectral absorptivities for bound-bound transitions, κ_ν^{bb}, the spectral absorptivity for bound-free transitions, κ_ν^{bf}, and the spectral absorptivity for free-free transitions, κ_ν^{ff}:

$$\kappa_\nu = \kappa_\nu^{bb} + \kappa_\nu^{bf} + \kappa_\nu^{ff}$$

The relations between the spectral absorptivities and the transition probabilities for these processes will be presented in Appendix C.

FIGURE 1

The equations relating the electrical power input to the optical radiation and thermal conduction.

(Saha's equation) and thus the electron density, and in broadening the lines through electron, ion, and Van der Waals mechanisms.

2.1 Electrical and Thermal Conductivity

The transport properties (i.e., the electrical and thermal conductivities) of partially ionized gases are currently under extensive investigation in many laboratories. We have used de Voto's calculations[9, 10] as applied to xenon using the momentum transfer cross section of Frost and Phelps.[11] The program for the electrical and thermal conductivities of xenon is given in Appendix A.

2 2 The Spectral Absorptivity

The spectral absorptivity of atomic species can now be calculated (in theory) to a relatively high precision without exorbitant computer time using "quantum defect" methods to obtain the transition probabilities for bound-bound transitions and the cross sections of the bound-free and free-free transitions. The electron broadening was calculated using the line broadening theory outlined by Griem[12] as applied by Corinaldesi.[13] Figure 2 shows schematically the calculation[3] of the spectral absorptivities which are carried out in appendices C and D and how they relate to the other programs.

The population of the initial level is one of the most important determinants of the strength of an absorption as the population in the initial level can vary in orders of magnitude as the temperature changes a few thousand degrees. If the line in bound-bound transition arises from a ground or very low lying state, the population in the level is very high in the cooler gas near the walls, thereby leading to a high spectral absorptivity. Examples for these ground state transition are the resonances lines of xenon lying in the vacuum ultraviolet and the yellow doublet of sodium. The high spectral absorptivity will be manifested in the arc discharge by very broadened and self reversed emission bands.

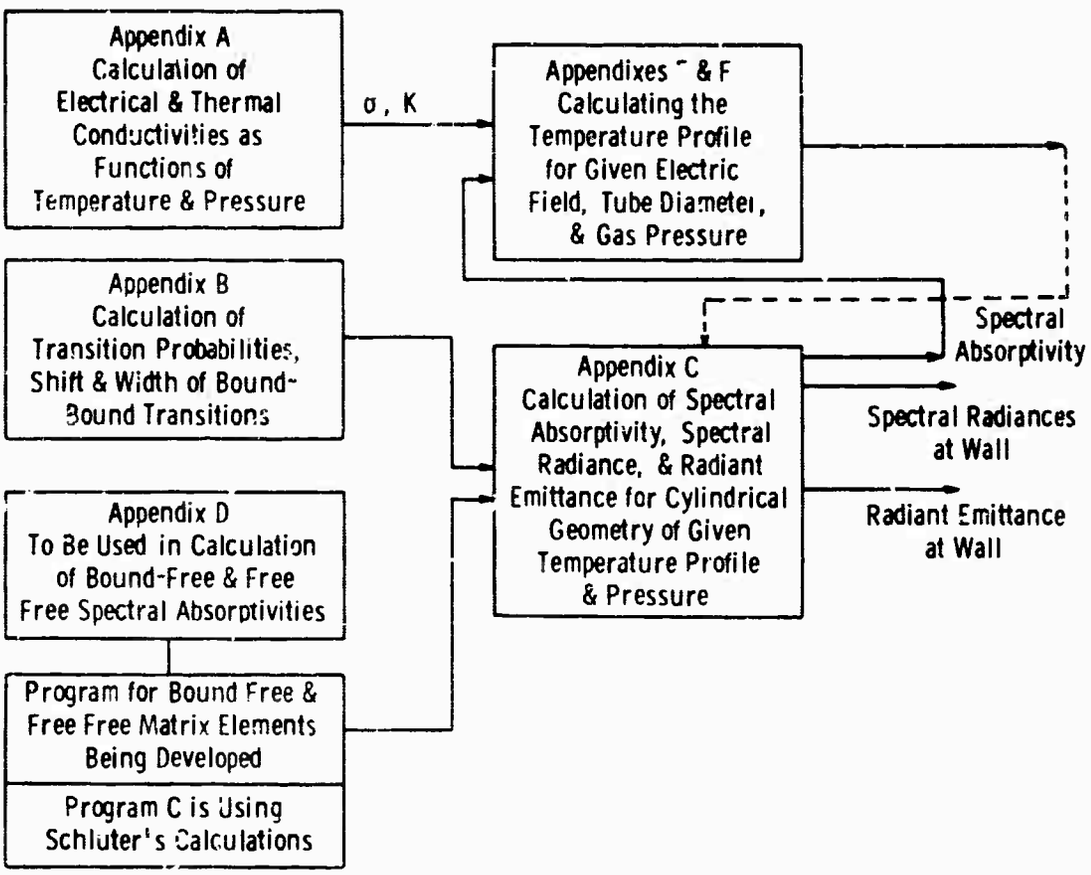

Fig. 2—The information flow for the calculation procedures in the appendixes

The shape of the line determines how the absorption varies with wavelength. We have considered the lines in the dense highly radiative plasmas treated herein to have a Lorentzian shape. The line width, w, and the shift, d, arises in the cases being considered from electron broadening in the center of the arc (Stark broadening theory), and neutral particle broadening near the edge (Van de Waals or resonance broadening).

The various broadening mechanisms are calculatable (in theory at least) for atomic systems such as xenon. Figure 3 shows the spectral absorptivities for xenon for a range of temperatures at the same pressure; 5 atm. The program for this is in Appendix C. The spectral absorptivities shown in Figure 3 include the broadened lines and the continuum. The lines were calculated using an intermediate coupling program described in the last report[4] and in Appendix B which was the extension to xenon of the calculation of Garstang and Van Blerkom.[14] The continuum was that calculated by Schluter[15] and is described in an earlier report and in Appendix C. The upper limit on the spectral absorptivities that may be calculated by this program is limited to below those temperatures for which Xenon II becomes appreciable (~ < 14,000°K) (We are modifying the programs to include XeII, but this work was not available for this report.) The effect of the XeII will be to increase the continuum and the emission in the blue and ultraviolet as XeII does not have the strong infrared lines that XeI exhibits.

2.3 The Arc Models

Two approaches were used in the creation of models for the arc. In the simplest, the arc was assumed to be homogeneous in temperature and thermal conduction to the walls was neglected. In the more complete approach, the absolute temperature profile is calculated for a given electric field and tube diameter. From the temperature profile, the spectral radiance through the arc, the radiation external to the arc, and the thermal conduction to the walls can be calculated.

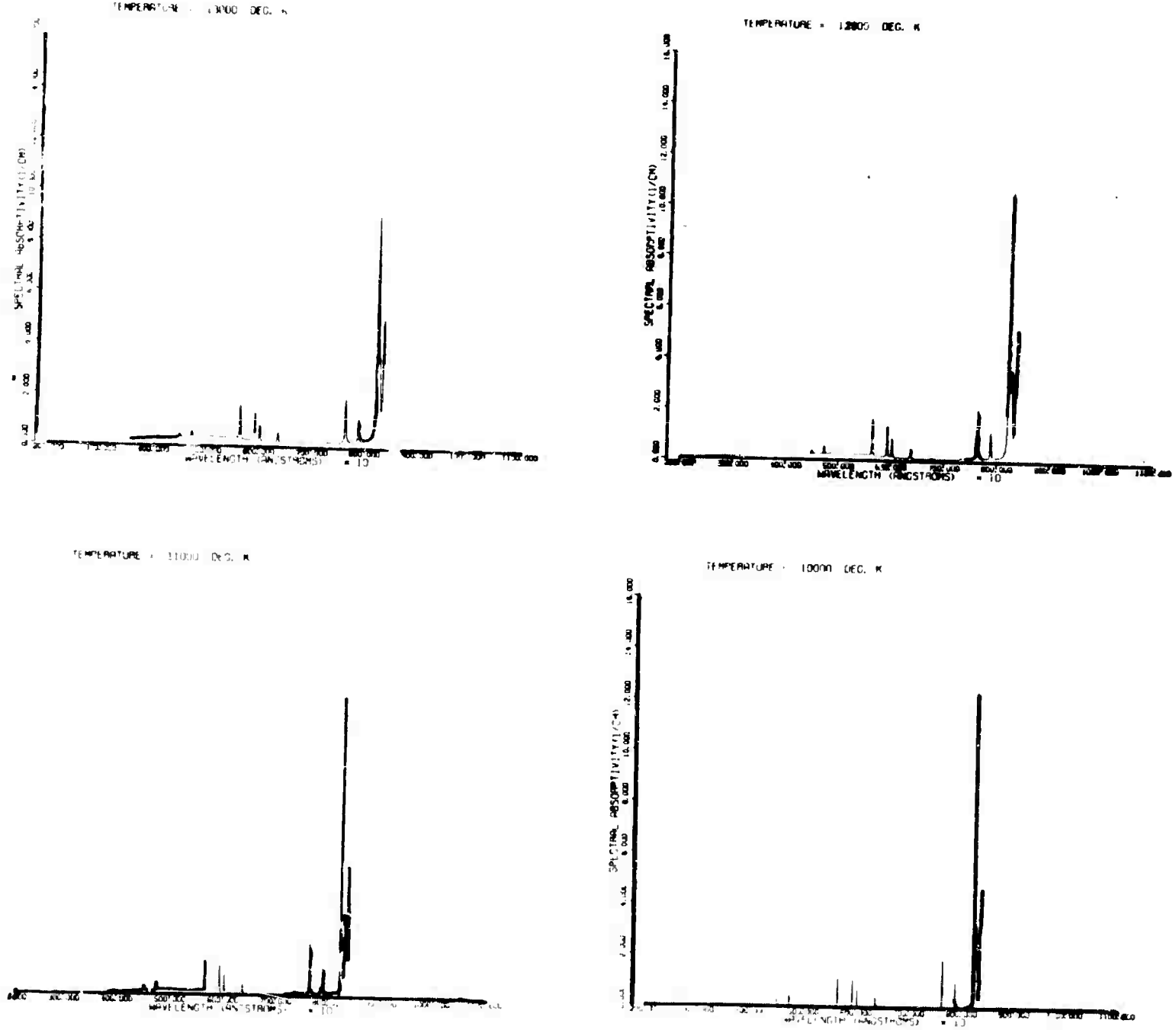

Fig. 3—The calculated spectral absorptivity of Xenon I over a range of temperatures for a pressure of 5 atm

The inclusion of the free-free transitions and the more complete calculations of the bound-free transitions required more extended application of the quantum detect methods of Seaton[16], and Burgess and Seaton[17]. Peach [18,19], Schlüter[15], and a series of papers by Biberman and Norman and their collaborators[20] have indicated improvements using the Coulomb field; Stewart and Rotenberg[21] and McGuire[22] have extended the theory to the non-Coulomb potential found in the inner part of the atom. The rise of these methods required programs for calculating Whittaker functions[23] of real and imaginary argument. Appendix D presents ALGOL translation of and corrections to the FORTRAN programs of McGuire[24]. These programs are to be used as entry points for the numerical integrations of the radial matrix elements for bound-free and free-free transitions.

The homogeneous temperature models considered the arc to be a cylinder of uniform temperature with the arc diameter to be an input parameter. The homogeneous temperature models for the pulsed arcs were found to give reasonable agreement with experiment if the arc diameter were properly chosen. In the previous report, the electrical conductivity determined from a .41 cm bore tube was used to calculate the arc core diameters for the larger tubes at the same temperatures using temperatures measured from a region of the spectrum that was assumed to be radiating like a black body. The radiant emittances (neglecting lines) calculated for the respective core diameters at the temperatures studied were found to account for the major portion of energy delivered to the flash tube.

The spectral radiance along a .8 cm diameter for a homogeneous temperature discharge of 12,000°A and 5 atm. is shown in Figure 4.

The spectral radiant emittances for two homogeneous temperature cylindrical arcs of .8 and 1.4 cm diameter are shown in Figure 5. The radiant emittance (i.e. radiative flux) is shown in the figure. The radiated power per unit length is simply the product of the radiant emittance and the surface area of the arc. The program for the calculation of the radiant emittance is part of Appendix C.

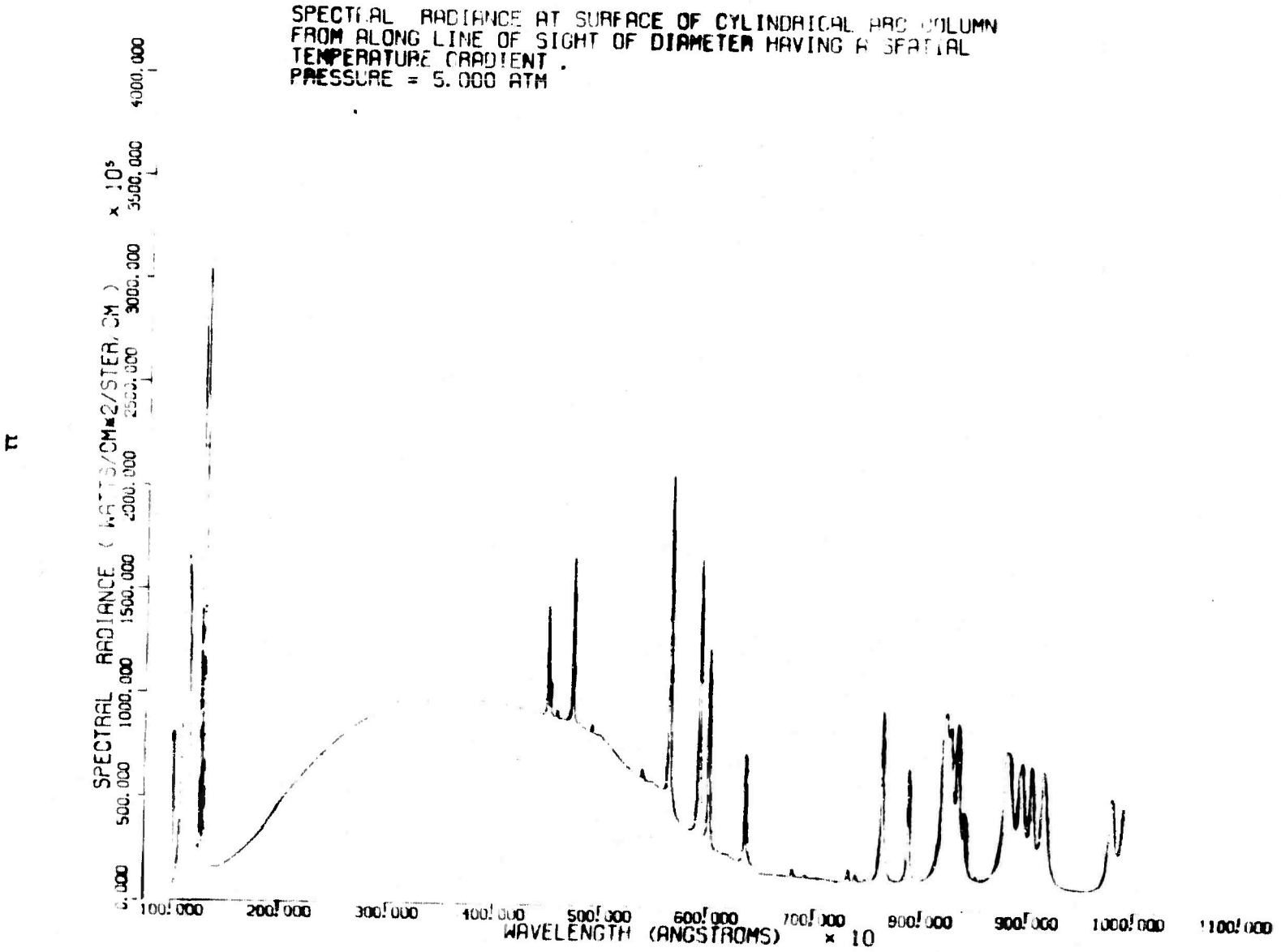

Fig. 4—The calculated spectral radiance along a .8 cm diameter homogeneous temperature Xenon plasma at 12000°K and 5 atm pressure

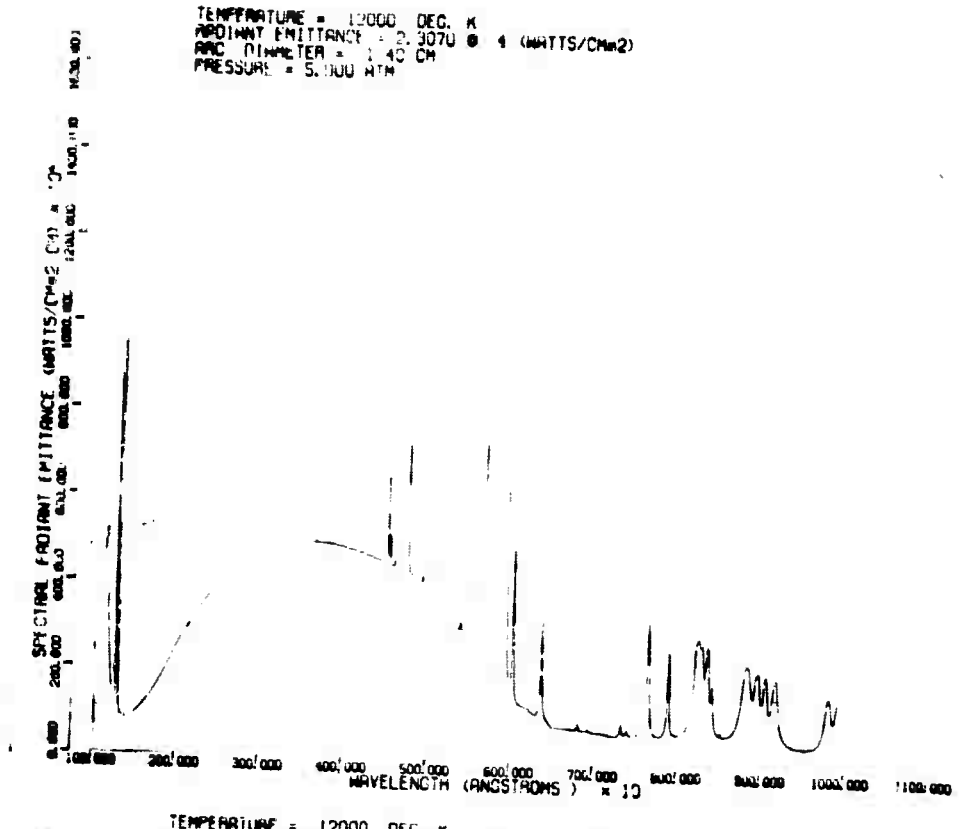

Fig. 5—The calculated spectral radiant emittances for .8 cm and 1.4 cm diameter homogeneous temperature cylindrical plasmas in Xenon at 12000°K & 5 atm pressure

The ideal model for the arc is one in which the characteristics of the arc discharge are determined by the input parameters: the electric field across the arc, the geometry of the arc container (i.e., the inside diameter of the cylinder), and the pressure and composition of the fill gas. But this model requires the solution to an integral-differential equation, called the energy balance equation, shown in part in Figure 1. The result of the application of the equation is simply the temperature distribution within the arc column.

We have explored a few methods for solving the energy balance equation for non-gray, nonhomogeneous plasma. The problem may be divided into two phases: determining the radiative flux (i.e., radiant emittance) throughout the arc column, and using the radiative flux together with the transport properties to find the temperature profile that satisfies the integral differential equation.

In this work, on Contract Nonr 4647(00), the radiative flux was calculated using an exact integration (described in Reference 2 and 25) and an approximate integration based upon a technique of Sampson[26]. The latter method was approximately ten times faster to compute than the former, and has given good agreement for the cases tested though it does not as yet include lines nor very steep ionization edges.

The temperature profile is calculated by using a relaxation method applied to the energy balance equation. In this, the radiative flux for an assumed (best guess) temperature profile is calculated. Using this radiative flux in a time dependent energy balance equation, the contributions of the other components of the energy balance equation are then calculated. By iterating the process over and over, a temperature profile that satisfies the equation could be calculated (i.e., where the time dependent part equals zero). This is described in Appendix E.

A program has been developed which combines the exact and approximate calculations to obtain a profile. The results of a sample calculation together with the program are given in Appendix E also.

To provide further insight into this calculation, an analysis procedure devised in other work[5] was applied to the xenon arc. The complete analysis together with calculated fluxes and temperature profiles is in Appendix F.

In all of these calculations, the pressure throughout the discharge is considered to be constant; that is, radiation and magnetic effects upon the pressure were neglected[1,2]. The gas pressure before the initiation of the discharge is known (typically, it is 150 to 300 torr for the xenon-filled flash tubes). Recent calculations have indicated that the final pressure in the fully developed arc is strongly dependent upon the temperature profile. A simple example will illustrate this dependence. Consider a simple two temperature confined arc in which the arc core is at 10,000°K, the volume near the walls is at 1000°K, and neglect the electron contribution to the pressure. It is simply shown that a cool arc volume of only 10% of the central core volume will reduce the arc pressure by a factor of two from the pressure that would occur if the central core occupied the whole volume as we had assumed in the earlier homogeneous temperature models[1,2,3]. This consideration in the pressure becomes very important for the larger diameters with larger cool portions[4].

III. COUPLING THE PUMP INTO THE LASER ROD

The ideal pump for optical lasers is one in which a major fraction of the energy radiated can be coupled or at least incident upon the laser rod. There are two general methods to do this: the diffusely reflecting cavity and the focussing cavity. We have investigated a particular diffusely reflecting cavity, the coaxial laser pump, which is well suited for use with large high energy pulsed laser, and a high image quality focussing system, the spherical cavity, which has demonstrated high efficiency in continuously operating laser systems[28].

Figure 6 shows a cross sectional drawing transverse to the rod of a current design coaxial lamp. The radiation from the plasma surrounds the laser rod. The MgO layer diffusely reflects the radiation back toward the laser rod. As Whittle and Skinner[29] point out, in a recent paper, the efficiency of the system may be obtained roughly by comparing the product of the area and energy absorbed by the rod with the sum of the products of areas and absorptions for the whole system. In this analysis

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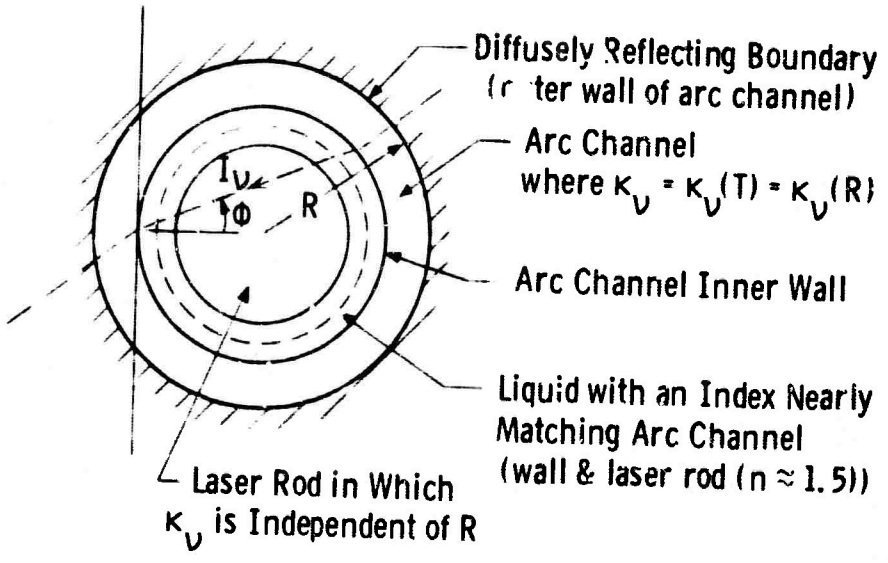

Fig 6—Simplified representation of laser rod-coaxial laser pump system

an open area is considered to be complete absorption. Good laser pump design would seek to minimize openings (as for electrodes) and minimize non-laser rod area. This line of reasoning is counter balanced partially by the need to minimize thermal conduction which varies with the gradient and may vary with plasma thickness. An unknown quantity in the analysis of an MgO reflector coaxial lamp is the reflectivity of the MgO layer under the conditions in the flash tube. This important parameter would need to be determined for a quantitative analysis of this pumping geometry.

Figure 7 is of a possible evolution of the coaxial laser pump which minimizes thermal losses, and allows very high energy outputs from energy limited laser rods. The minimizing of the thermal losses arises from the reduction per unit laser rod area of absorbing diffusely reflecting surfaces and of thermally conducting walls

To date our efforts on the use of the spherical cavity have been with small rods though the geometry need not be limited to them. Figure 8 from Reference 28 shows the geometry of the spherical cavity with the laser rod and laser pump symetrically disposed about the radius of curvature. If the laser rod length is small enough relative to the diameter of this sphere (and the spherical mirrors are of optical quality), the image of the lamp can be placed upon the rod for a very large fraction of the total solid angle. The data we have at present were obtained on 3 x 30 mm laser rods in which were obtained an efficiency of 1.15% and a total power of 3.6 watts for a Nd:YAG rod with external resonators. The application of this high efficiency system to larger laser rods is underway.

The spherical cavity has many advantages for laser pumping and a major disadvantage, this being the size sphere required for a rod of a given length (the diameter of the sphere should be considerably larger than the rod length). Some of the advantages include a high transfer efficiency (that can be calculated and ray traced readily), and a relatively remote reflecting surface (less subject to radiation damage).

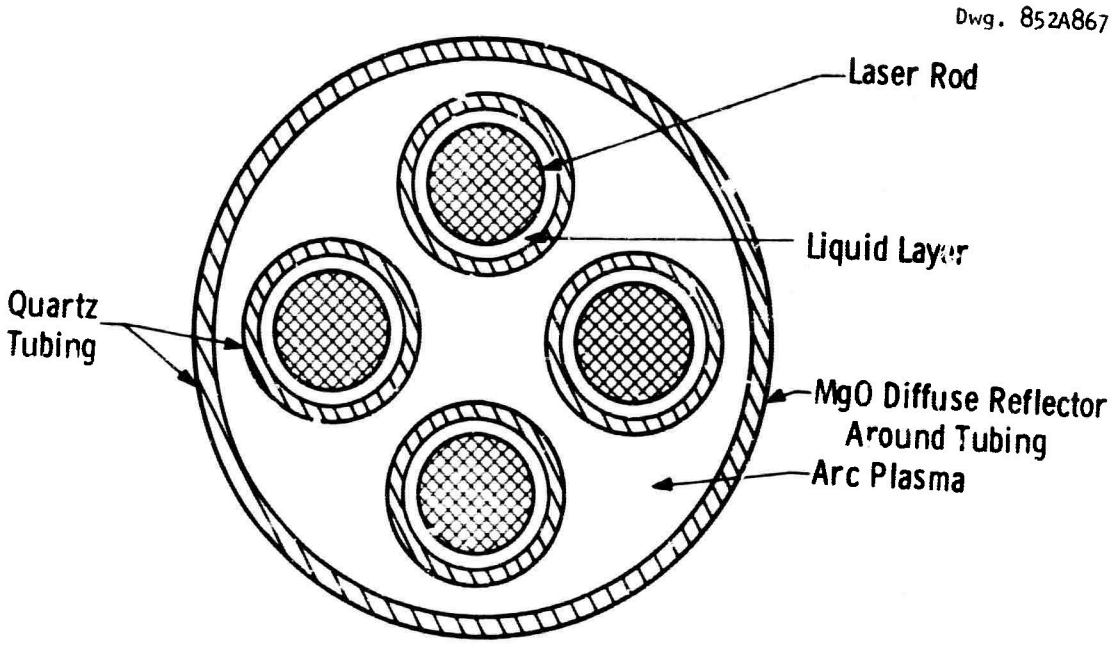

Fig. 7—Multiple rod coaxial laser pump

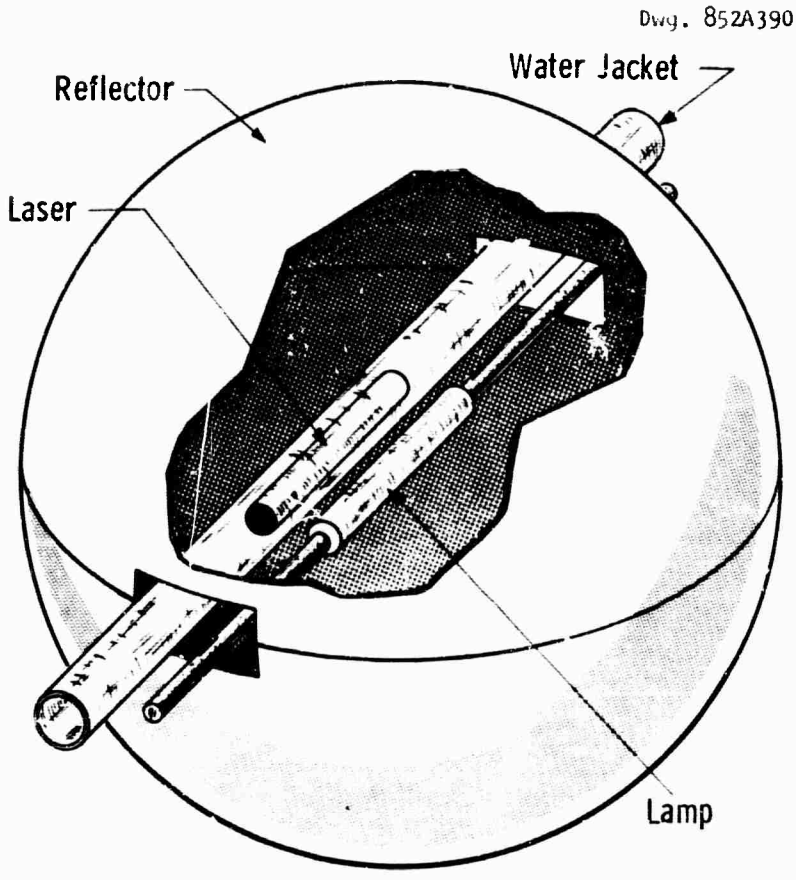

Fig. 3–Geometry of the spherical reflector

The sphere may be fabricated in large sizes readily to optical tolerances. The results obtained with the spherical cavity indicate promise for use in high energy laser pumping.

IV. RECENT EXPERIMENTAL MEASUREMENTS ON THE ARC

The experimental measurements taken throughout this work have been directed towards improving and verifying the information used in th models. Early in the work, we developed a technique to measure the temperature of the plasma (More correctly we developed a technique to measure the lower bound of the temperature - we will treat this more thoroughly in the discussion in double pulsed arcs). To calculate the spectral properties, we needed to know the pressure in the discharge. As we had the initial pressure of the gas (typically 150 torr) and the arc filled the tube to a first approximation, we initially assumed a homogeneous temperature. The arc was measured from the radial distribution of the spectral radiance in the ultraviolet to be relatively homogeneous for a large fraction of the radius - though subsequent estimates from the electrical conductivity discussed in the last semi-annual report[4] indicated this fraction varied with flash tube inside diameter. Recent analysis of the effect upon the pressure of the temperature profile within the tube indicated that measurements of the pressure or the electron density were required.

The experimental work in the past few months has been concerned with measurements of the pressure using a piezoelectric transducer, a Kistler Instrument Co. 603A, and of the spectral radiance in the vicinity of some lines and in various continuum regions for the arc under power densities over 1.5 MW/cm^3 (using pulse preionization[7]). Measurements were also made of the spectral radiance in the ultraviolet (at 3000Å) for the arc viewed side in and viewed end on. These measurements from the side and end would give a path length difference of ten or more depending upon the tube.

The pressure measurements for the 12.7 and 19 mm inside diameter tubes had shown a pressure considerably lower than that calculated for a homogeneous temperature distribution. The transducer output was very oscillatory reducing the accuracy. These measurements indicated that there was a cool volume near the walls which could change considerably during the arc cycle. A laser interferometer is being set up to measure the electron density in the center of the arc, but no final results are available for this report. The interferometer is similar to that of Gerardo et. al.[8] in which the flash tube is inside a reference cavity which is in series with the laser cavity. Measurements of the electron density with the interferometer together with those of temperatures will characterize more fully the arc plasma.

The measurements of the temperature in the double pulsed arc required finding spectral regions in which the emission from the arc was not self-reversed but still optically thick. The 8231.6A line of XeI was suspected to be self-reversed at power densities above about .1 MW/cm^3. This was confirmed using the high resolution rapid scanning spectrometer[6]. Calculations of the spectral radiance (using the program in Appendix C) for a temperature profile similar to that expected in the arc showed self reversal in the immediate vicinity of the 8231.6 Å lines.

The spectral radiances measured for the lines and the continuum are shown in Figures 9 through 12 for power densities over 1.5 MW/cm^3. In Figures 9 and 10, the spectral radiance is plotted in terms of the equivalent black body temperature. The power is the input power dissipated in the lamp per unit volume. The flash tube diameters ranged from .41 cm to 1.94 cm. The tubes were preionized with a .5 ms pulse (100-600 μF in series with 100 μHy). The main pulse was about 50 μs long (50-100 μF and the residual inductance ~3μH). The main pulse was switched in by means of an ignitron using the circuit shown in Reference 6. The self reversal of the 8231.6 Å line of XeI was considered to be the primary reason for the reduction in the spectral radiances for the larger diameter flash tubes. Figure 13 gives the spectral radiance distribution for an EG & G Inc. FX-52 flash tube under single and double pulsed conditions. The data was taken with a spectral width of about 1 Å at the wavelengths indicated.

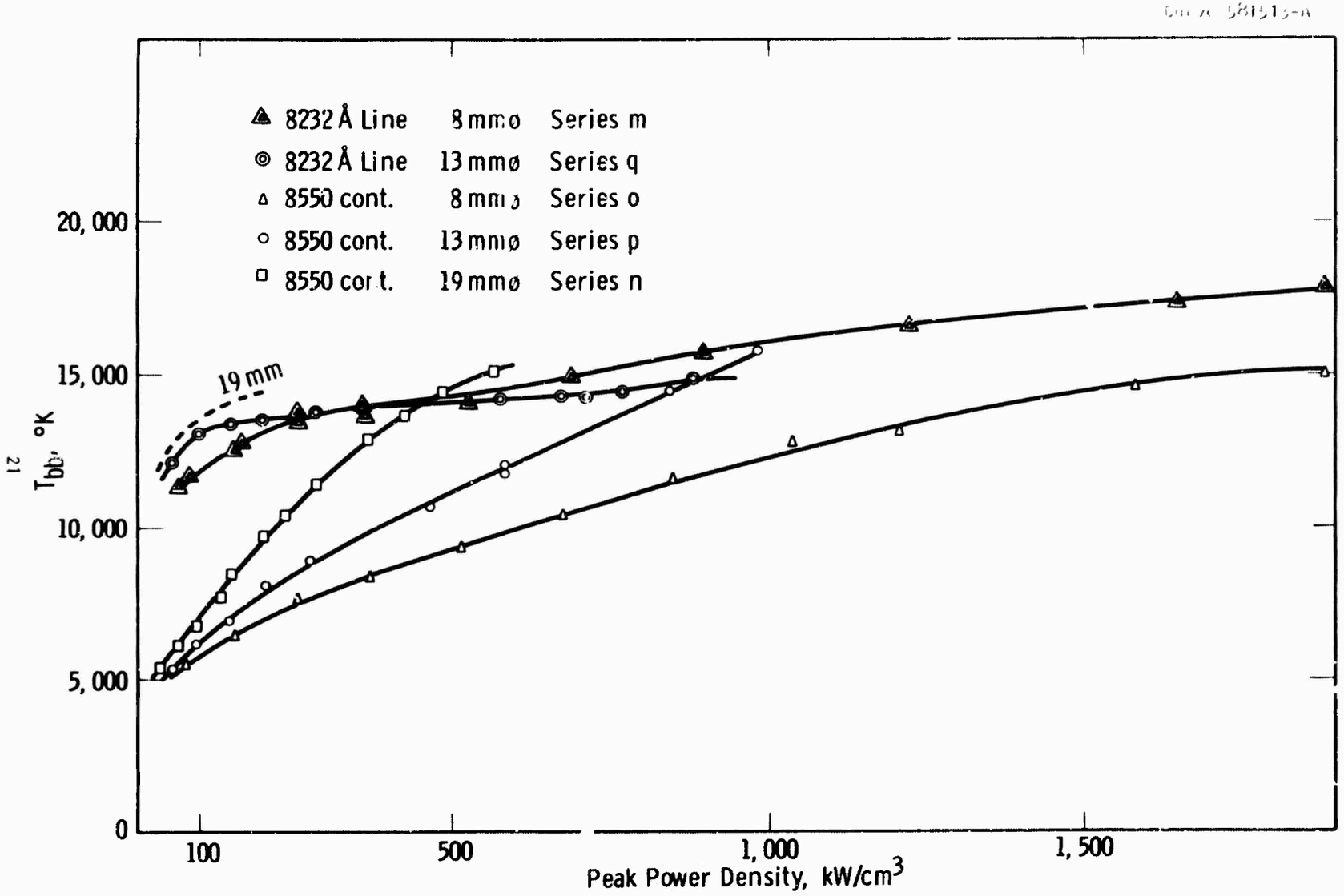

Fig. 9—Black body temperature corresponding to measured spectral radiance as a function of input power density

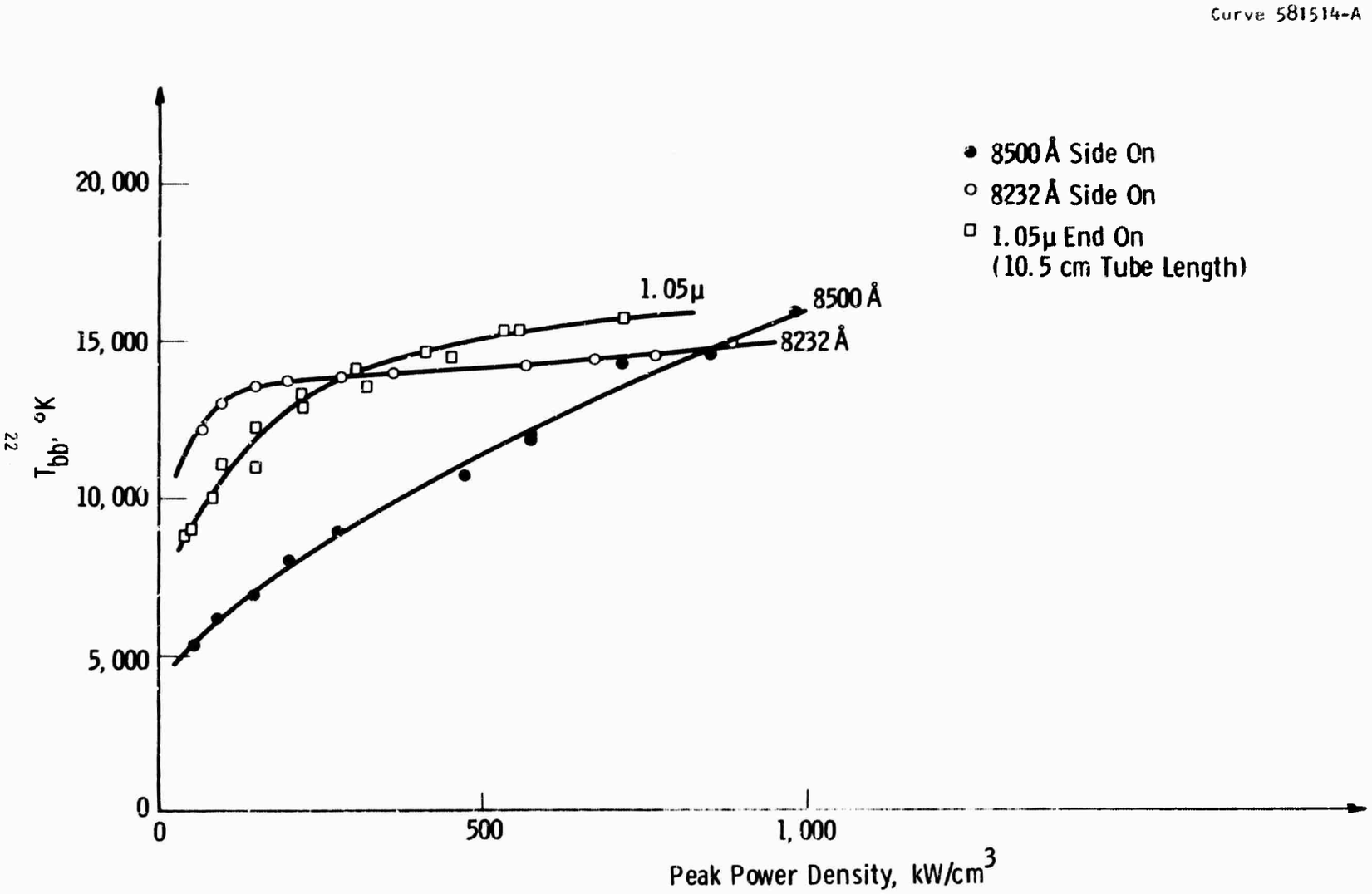

Fig. 10—Black body te nperature corresponding to same spectral radiance as 13 mm flash tube as a function of input power density

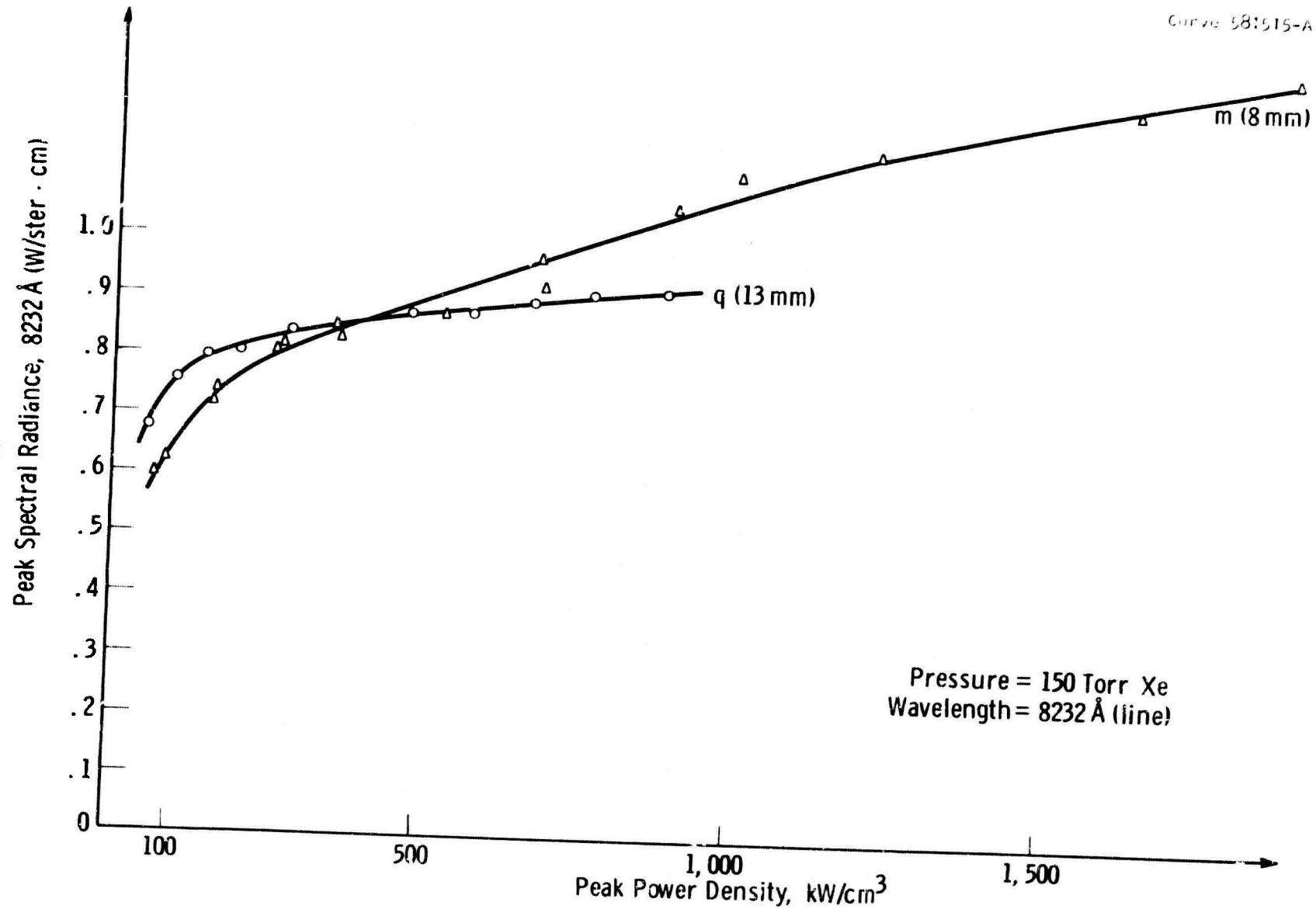

Fig. 11—Spectral radiance of linear cylindrical Xe flash tubes of different diameters as a function of power density input

Fig. 12—Spectral radiance of linear cylindrical Xe flash tubes of different diameters as a function of power input

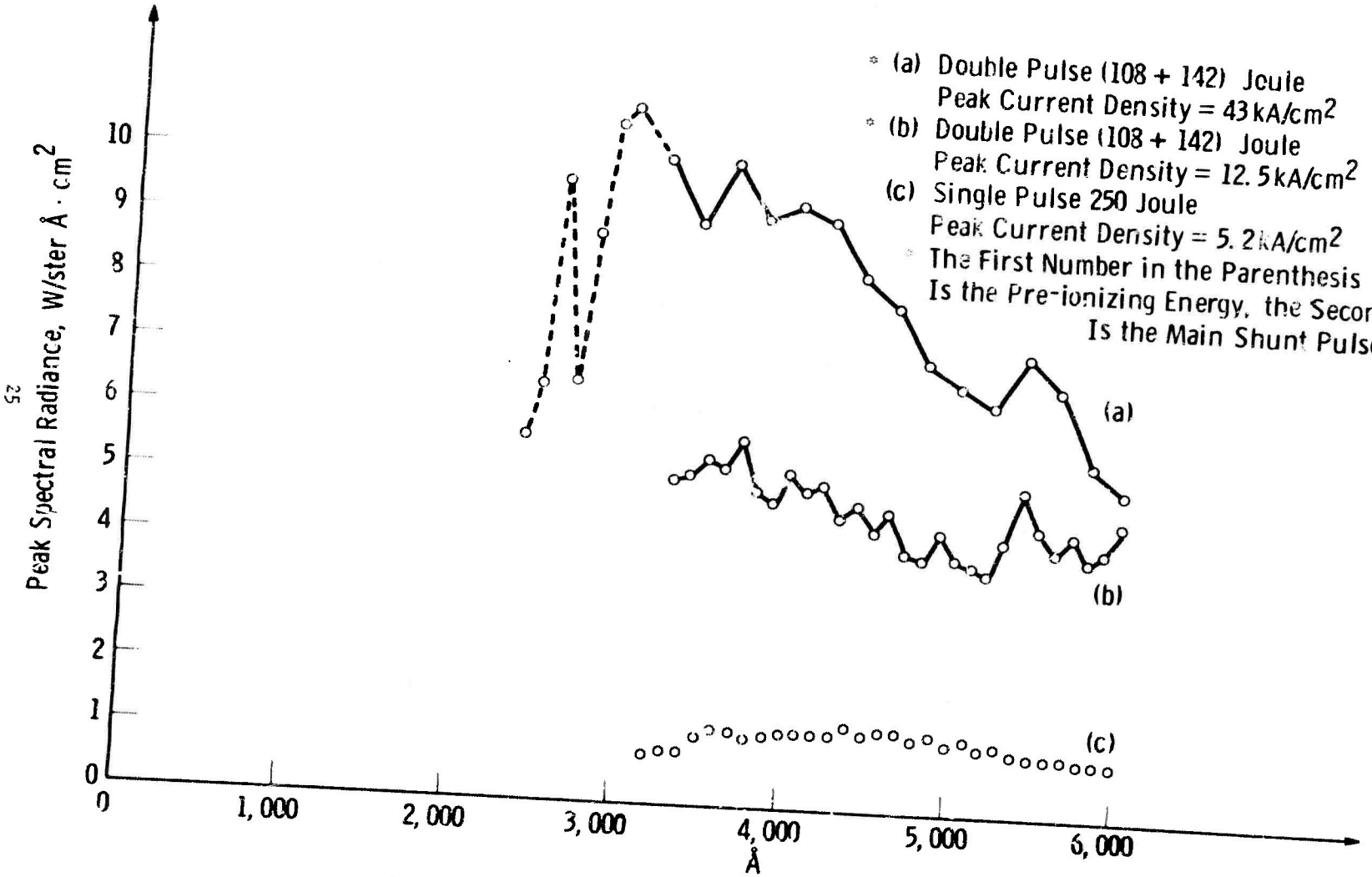

Fig. 13—Spectral radiance distribution for an EG & G Inc. FX-52 flash tube single & double pulsed

The measurements of the spectral radiance at 3000 Å on flash tubes viewed side on and viewed end on yielded the theoretical ratio of the length of the tube to diameter of the tube for lower energies only when the tungsten electrodes were moved back out of the arc. The ratio again deviated at the higher currents as shown in Figure 14. This may arise in part from further tungsten injection, but also may be due to the plasma becoming thick for the flash tube length being viewed.

We have not yet made a detailed comparison of the calculated radiances with those measured experimentally. This requires a more accurate knowledge of the pressure and/or the electron density than we currently have. We shall be making these comparisons after the laser interferometer is completed. To compare the spectral radiances observed in Figure 13 with the calculated values in Figure 4, multiply the values in Figure 13 by 10^8 to obtain the values in Figure 4 (W/cm^2 Ster cm). The single pulsed values correspond with those for the plot in Figure 4; the exact agreement requiring better values of pressure than we currently have.

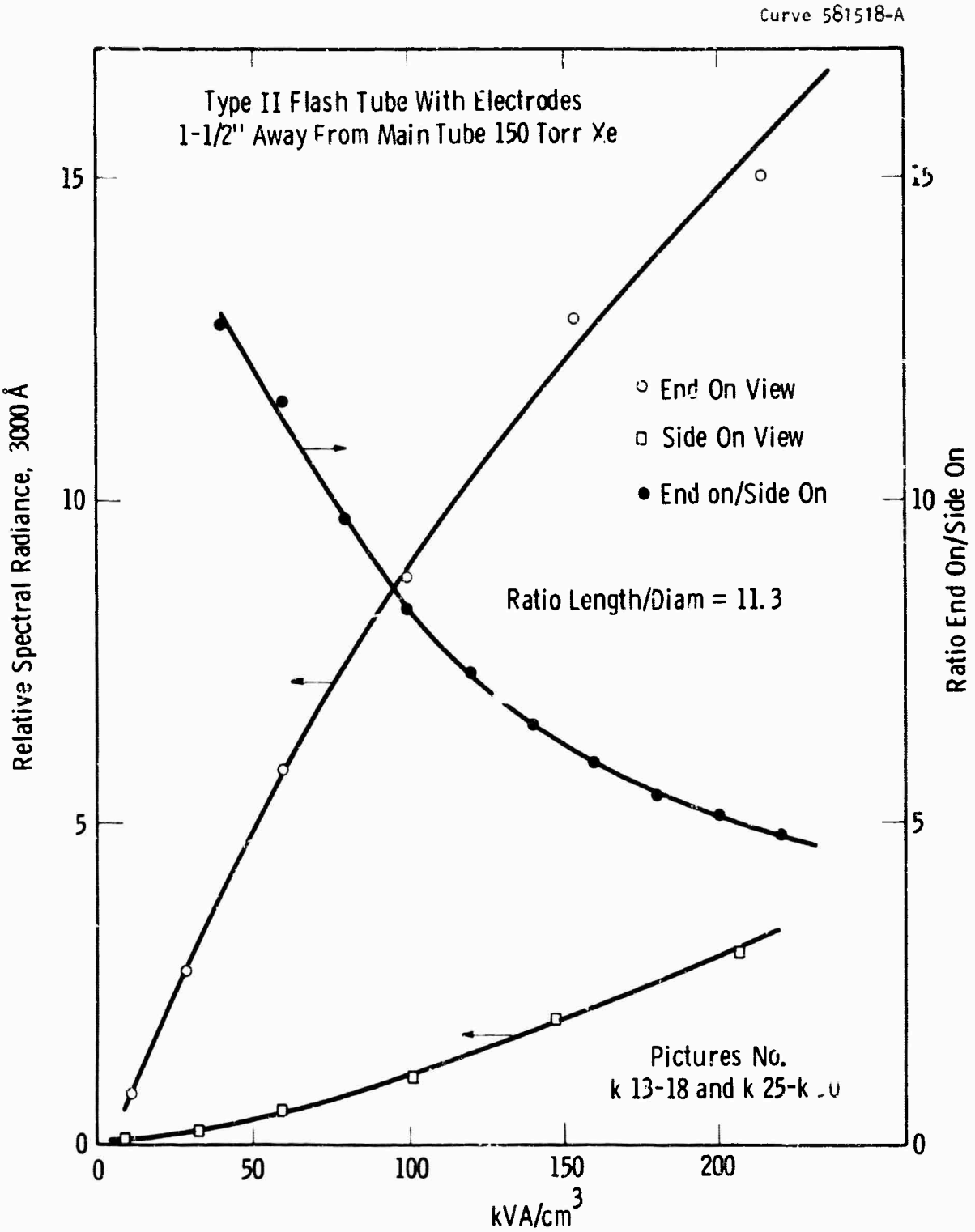

Fig. 14—The spectral radiance viewed at 3000 Å end on and side on for a 13 mm diameter arc tube

V. SUMMARY AND CONCLUSIONS

This report presents a description of the work carried out on Contract Onr 4647(00) towards the creation of quantitative models for the pulsed arc discharge that is used for the optical pumping of high energy solid state lasers. The primary results of these studies are computer programs for the calculations of the physical properties of the arc plasma, using xenon as the working gas, and for determining the balance within the arc between radiation external to the arc and thermal losses to the walls. The experimental results obtained since the last semiannual reports are also described. The experimental studies have been concerned with measurements of the pressure within the arc, and the characterization of the arcs at very high power densities.

The models for the arc developed in this work are at present only semi-quantitative. They possess the main features of the arc, exhibiting the saturation of the radiation in the infrared, the strong dependence upon power density of the radiation emitted in the ultraviolet; and the nearly homogeneous temperature distribution that have been observed in these arcs. To improve the accuracy of the models, more complete and accurate measurements of the physical properties need to be made. Through the use of the model calculations, quantitative comparisons can be made between the power input, the average electrical conductivity, the spectral absorptivities in various regions of the continuum and in the vicinity of selected lines, and of the pressure and electron density to make a consistent picture.

The full implications of these models are still being explored. The models are allowing a new insight into the behavior of the high density arc. The arc models help to remove the high density plasma - the light emitting plasmas - from the "art" area of technology.

We hope that the work described in this series of reports will assist the designer of optically pumped lasers in the development and improvement of this area of laser technology.

Through this work, we hope that we are bring to bear on an old problem-- light sources--some of the new techniques in both theory and experiment that were developed by a wide variety of people working in areas far removed from the optical pumping of lasers.

VI. ACKNOWLEDGMENTS

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APPENDIX A

A PROGRAM FOR THE CALCULATION OF THE ELECTRICAL AND THERMAL CONDUCTIVITY OF XENON AS A FUNCTION OF TEMPERATURE AND PRESSURE

by

R. S. deVoto
Stanford University

This program, ELEC/THERM, calculates the various components of the electrical and the thermal conductivities of xenon as a function of pressure and temperature under local thermal equilibrium conditions.

The program will calculate these quantities for argon also. The input data for argon is:

1. "ARGON", number of species - 1 (we used 2)
2. initial temperature, temperature step size, maximum temperature desired
3. number of pressures; the pressures in atmospheres
4. PHIOA (3.23 @ 4), RHOA (.224), PHIOI (5.38 @ 6), RHOI (.1965), AC (25.615), BC (1.1960), HIER (must be 0).
5. electron mass (9.1091 at -28), molec. wt. of atom (39.944), molec. wt. of first ion (39.944), molec. wt. of any other ions used.

For xenon the data required is similar to the ARGON program.

1. "XENON", 2,
2. initial temperature, step size, maximum temperature desired
3. number of pressures, the pressures (in atmospheres)
4. 3.11 @ 6, .208,0,0, 25.639, .99752,0, 9.109 @ -28, 131.3,131.3.

```
BEGIN                                                                                SC   1:   010
                                                                START OF SEGMENT ********** 0002
COMMENT  THIS PROGRAM PUNCHES THE FOLLOWING CARDS:                                   SC   2:   010
INITIAL TEMPERATURE,STEP SIZE,FINAL TEMPERATURE                                      SC   2:   010
FOR EACH PRESSURE:                                                                   SC   2:   010
PRESSURE (IN ATMOSPHERES)                                                            SC   2:   010
ELECTRICAL CONDUCTIVITIES FOR ALL TEMPERATURES FOR THIS PRESSURE                     SC   2:   010
THERMAL CONDUCTIVITIES FOR ALL TEMPERATURES FOR THIS PRESSURE                        SC   2:   010
;                                                                                    SC   2:   010
COMMENT CLOSEDECK;                                                          00000000 SL   2:   010
                                                                            99999999 SC   2:   010
FILE IN READER(2,10);                                                                SC   2:   010
FILE OUT OFIL 6(2,15);                                                               SC   2:   312
FILE OUT PUNCH DISK SERIAL [20:650] (2,10,30,SAVE 1);                                SC   2:   710
INTEGER NP,IP,IT;                                                                    SC   2:  1012
REAL T1,DT,TMAX;                                                                     SC   2:  1012
ARRAY PP[0:30];                                                                      SC   2:  1012
ARRAY TEMP,THEAVY,TELEC,TREACT,TTOT,SIGMA[0:190];                                    SC   2:  1211
 REAL DEBYE,ELEC,PSI,LAMBDA ;     REAL ARRAY Q[0:3,0:5,0:5,0:5] ;           NES 0001 SC   2:  1511
 REAL T,P,       LMBDA,NTOT,ALF ;                                                    SC   2:  1712
 INTEGER MAX,I,J ;                           ALPHA NAM ;                             SC   2:  1712
 REAL ARRAY N[0:5] ;                                                                 SC   2:  1713
 FORMAT FP( "TRANSPORT PROPERTIES OF ",A6," AT P =",F6.2," ATMOS,"),                 SC   2:  1012
                                                                START OF SEGMENT ********** 0010
    CLOCK("PROCESSOR TIME USED IS",R9.2," SECONDS",                                  SC  10:  1012
          "I/O TIME IS",R9.2," SECONDS"),                                            SC  10:  1012
    PUNCHO(5(E12.5,",")),                                                            SC  10:  1012
    PUNCHSTAR("*,"),                                                                 SC  10:  1012
       F1(/"T=",F7.0,X1,3("N(",I1,")=",E10.3,X1),"ALPHA=",F10.3,/                    SC  10:  1012
       "DEBYE=",E10.3,X1,                                                            SC  10:  1012
          "ELEC=",F10.3,X1,"LAMBDA=",E10.3,X1,  "SIGMA=",E10.3,X1,                   SC  10:  1012
          "LMBDA=",E10.3 ) ;                                                         SC  10:  1012
                                                               0010 IS 0072 LONG, NEXT SEG 0002
 PROCEDURE SAHA ( T,P,ALFA ) ;    COMMENT XENON ;                           SAHA0010 SC   2:  1012
    VALUE T,P ;     REAL T,P,ALFA ;                                         SAHA0020 SC   2:  1012
    BEGIN    REAL X,ZA,ZI ;                                                 SAHA0030 SC   2:  1012
                                                                START OF SEGMENT ********** 0011
    X ← 97834.4/ T ;                                                        SAHA0040 SC  11:   010
    IF X > 110 THEN ALFA ← 0                                                SAHA0050 SC  11:   111
    ELSE  BEGIN                                                             SAHA0060 SC  11:   213
    ZA ← 1 ;                                                                SAHA0070 SC  11:   510
    ZI ← 4 + 2 × EXP(-15160.96/ T) ;                                        SAHA0080 SC  11:   513
       ALFA ← 1 / SQRT(1 + 1999.6 × P × ZA ×(EXP(X)/(T*2.5×ZI))); END;      SAHA0090 SC  11:   813

 END SAHA ;                                                                 SAHA0100 SC  11:  1611
                                                               0011 IS 0022 LONG, NEXT SEG 0002
PROCEDURE QEXE( T,I,J ) ;    COMMENT VERSION 2/24/66; THIS INCLUDES THE     QEXE0001 SC   2:  1012
 CROSS SECTIONS AS COMPUTED FROM FROST & PHELPS DATA-TO 5*5 ONLY ;          QEXE0002 SC   2:  1012
    VALUE T,I,J ;       REAL T ;     INTEGER I,J ;                          QEXE0003 SC   2:  1012
 BEGIN                                                                      QEXE0004 SC   2:  1012
    OWN INTEGER K ;        OWN REAL ARRAY II[0:6,0:39] ;                    QEXE0005 SC   2:  1012
                                                                START OF SEGMENT ********** 0012
    INTEGER S,K1,K2 ;     REAL C1,C2,C3,THETA ;      LABEL L1,L2 ;          QEXE0006 SC  12:   213
    FORMAT F1( 10("*"),"T =",F6.0," IS OUT OF RANGE OF QARG()" /) ;         QEXE0007 SC  12:   213
                                                                START OF SEGMENT ********** 0013
                                                               0013 IS 0014 LONG, NEXT SEG 0012
    IF K = 0 THEN  BEGIN                                                  - QEXE0008 SC  12:   213
    FILL II[0,*] WITH                                                       QEXE0009 SC  12:   410
      21.627,  9.617,  5.568,  3.940,  3.332,  3.241,  3.454,  3.863,       QEXE0010 SC  12:   413
                                                                START OF SEGMENT ********** 0014
       4.410,  5.055,  5.773,  6.544,  7.352,  8.193,  9.027,  9.875,       QEXE0011 SC  12:   610
      10.718, 11.552, 12.371, 13.172, 13.952, 14.707, 15.438, 16.142,       QEXE0012 SC  12:   610
      16.819, 17.469, 18.092, 18.687, 19.256, 19.798, 20.314, 20.805,       QEXE0013 SC  12:   610
      21.271, 21.714, 22.134, 22.332, 22.900, 23.265, 23.601, 23.919;       QEXE0014 SC  12:   610
                                                               0014 IS 0080 LONG, NEXT SEG 0012
    FILL II[1,*] WITH                                                       QEXE0015 SC  12:   610
      16.267,  5.401,  3.105,  2.615,  2.833,  3.411,  4.209,  5.158,       QEXE0016 SC  12:   613
                                                                START OF SEGMENT ********** 0015
       6.213,  7.341,  8.515,  9.711, 10.912, 12.099, 13.242, 14.390,       QEXE0017 SC  12:   810
      15.476, 16.516, 17.505, 18.442, 19.327, 20.159, 20.939, 21.669,       QEXE0018 SC  12:   810
      22.349, 22.983, 23.572, 24.117, 24.622, 25.088, 25.517, 25.911,       QEXE0019 SC  12:   810
      26.272, 26.603, 26.906, 27.177, 27.425, 27.648, 27.849, 28.027;       QEXE0020 SC  12:   810
                                                               0015 IS 0080 LONG, NEXT SEG 0012
    FILL II[2,*] WITH                                                       QEXE0021 SC  12:   810
       9.932,  3.353,  2.280,  2.569,  3.373,  4.466,  5.753,  7.174,       QEXE0022 SC  12:   813
                                                                START OF SEGMENT ********** 0016
       8.680, 10.229, 11.784, 13.315, 14.799, 16.219, 17.563, 18.823,       QEXE0023 SC  12:  1010
      19.996, 21.082, 22.081, 22.997, 23.832, 24.591, 25.278, 25.896,       QEXE0024 SC  12:  1010
      26.455, 26.953, 27.397, 27.791, 28.137, 28.441, 28.706, 28.931,       QEXE0025 SC  12:  1010
      29.123, 29.284, 29.414, 29.521, 29.601, 29.658, 29.694, 29.711;       QEXE0026 SC  12:  1010
                                                               0016 IS 0080 LONG, NEXT SEG 0012
    FILL II[3,*] WITH                                                       QEXE0027 SC  12:  1010
       7.199,  2.366,  2.196,  3.052,  4.343,  5.908,  7.640,  9.527,       QEXE0028 SC  12:  1013
                                                                START OF SEGMENT ********** 0017
      11.441, 13.348, 15.189, 16.982, 18.581, 20.092, 21.471, 22.718,       QEXE0029 SC  12:  1210
      23.837, 24.834, 25.717, 26.494, 27.177, 27.770, 28.281, 28.719,       QEXE0030 SC  12:  1210
      29.090, 29.400, 29.655, 29.860, 30.019, 30.138, 30.220, 30.268,       QEXE0031 SC  12:  1210
      30.286, 30.277, 30.242, 30.185, 30.107, 30.011, 29.899, 29.771;       QEXE0032 SC  12:  1210
                                                               0017 IS 0080 LONG, NEXT SEG 0012
```

```
     FILL I1[4,*] WITH                                                          QEXE0033 SC  12;  121C
        5.183,  1.950,  2.456,  3.795,  5.546,  7.570,  9.786, 12.062,          QEXE0034 SC  12;  1213
                                                                   START OF SEGMENT ........... 001P
       14.317, 16.478, 18.494, 20.340, 21.996, 23.465, 24.752, 25.869,          QEXE0035 SC  12;  141C
       26.831, 27.651, 28.344, 28.924, 29.402, 29.789, 30.094, 30.332,          QEXE0036 SC  12;  141C
       30.504, 30.620, 30.684, 30.707, 30.690, 30.637, 30.553, 30.442,          QEXE0037 SC  12;  141C
       30.306, 30.149, 29.972, 29.779, 29.571, 29.350, 29.117, 28.874;          QEXE0038 SC  12;  141C
                                                                   0018 IS 0040 LONG, NEXT SEG 0012
     END ;                                                                      QEXE0039 SC  12;  141C
     K ← ENTIER( T/500 - .5) ;                                                  QEXE0040 SC  12;  141C
     IF T < 750 OR T >10750 THEN     BEGIN                                      QEXE0041 SC  12;  1413
WRITE(GEIL,F1,T);                                                                        SC  12;  191C
        GO TO L1 ;     END ;                                                    QEXE0043 SC  12;  2411
     THETA ← T - 500 × (K + 1) ;                                                QEXE0044 SC  12;  2513
     IF ABS(THETA) < 20 THEN  GO TO L1 ;                                        QEXE0045 SC  12;  311C
        K1 ← K -1 ;                                                             QEXE0046 SC  12;  3212
        K2 ← K +1 ;                                                             QEXE0047 SC  12;  3313
        THETA ← THETA / 500 ;                                                   QEXE0048 SC  12;  351C
        C1 ← THETA × (THETA - 1) / 2 ;                                          QEXE0049 SC  12;  3611
        C2 ← 1 - THETA × THETA ;                                                QEXE0050 SC  12;  3812
        C3 ← THETA × (THETA + 1) / 2 ;                                          QEXE0051 SC  12;  4011
        FOR S ← 0 STEP 1 UNTIL 8 DO                                             QEXE0052 SC  12;  4212
           Q[1,S+1,I,J]←C1×I1[S,K1] + C2×I1[S,K] + C3×I1[S,K2] ;               QEXE0053 SC  12;  441C
        GO TO L2 ;                                                              QEXE0054 SC  12;  5513
L1:     FOR S ← 1 STEP 1 UNTIL 8 DO                                             QEXE0055 SC  12;  5611
           Q[1,S,I,J] ← I1[S-1,K] ;                                             QEXE0056 SC  12;  581C
L2:                                                                             QEXE0057 SC  12;  6511
END QEXE ;                                                                      QEXE0058 SC  12;  661C
                                                                   0012 IS 0072 LONG, NEXT SEG 0002
PROCEDURE QEXP(RHIO,RHO,T,I,J);COMMENT VERSION 8/28/65 ;VALUE RHIO,RHO,T        QEXP0010 SC   2;  1012
,I,J;REAL RHIO,RHO,T;INTEGER I,J;BEGIN COMMENT RHIO IN E.V.,RHO IN ANGST        QEXP0020 SC   2;  1012
ROMS ;INTEGER K,K1,K2;OWN INTEGER KK;OWN REAL ARRAY AA[0:60],I22[0:60];R        QEXP0030 SC   2;  1012
                                                                   START OF SEGMENT ........... 0015
EAL A0,DA,DA1,C1,C2,C3;LABEL INTERP;FORMAT F1(10("*"),"A0=",F8.3," IS OU        QEXP0040 SC  19;   812
                                                                   START OF SEGMENT ........... 0020
T OF RANGE OF QEXP")/);IF KK=0 THEN BEGIN FILL AA[*] WITH 3,3.5,3.75,4,4.2      QEXP0050 SC  20;   812
                                                                   0020 IS 0018 LONG, NEXT SEG 0015
                                                                   START OF SEGMENT ........... 0021
5,4.5,4.75,5,5.25,5.5,5.75,6,6.25,6.5,6.75,7,7.25,7.5,7.75,8,8.25,8.            QEXP0060 SC  19;   712
5,8.75,9,9.5,10,10.5,11,11.5,12,12.5,13,13.5,14,14.5,15,15.5,16,                QEXP0070 SC  19;   712
16.5,17,18,19,20,21,22,23,24,25,26,27,28,28.5;FILL I22[*] WIT                   QEXP0080 SC  19;   712
                                                                   0021 IS 0051 LONG, NEXT SEG 0015
H,503325,.506273,.508652,.510658,.512247,.513587,.514665,.515543,.516255        QEXP0090 SC  19;   81C
                                                                   START OF SEGMENT ........... 0022
,.516829,.517284,.517646,.517924,.518133,.518258,.518384,.518445,.518449        QEXP0100 SC  19;   911


,.518463,.518431,.518375,.518306,.518218,.518005,.517758,.517477,.517152        QEXP0110 SC  12;   911
,.516877,.516565,.516251,.515937,.515626,.515319,.515017,.514723,.514430,       QEXP0120 SC  12;   911
.514147,.513603,.513057,.5126,.512141,.511708,.511290,.510914,.510551,.5        QEXP0130 SC  12;   911
10205,.509884,.509578,.509287,.509108;KK←25;END;A0←LN(RHIO/(8.4147@-5×T)        QEXP0140 SC  12;   911
                                                                   0022 IS 0050 LONG, NEXT SEG 0015
)/A0←A0-AA[KK];DA1←ABS(DA);IF DA1<.125THEN GO TO INTERP ELSE IF DA<0THEN        QEXP0150 SC  10;  1011
 BEGIN K1←-1;K2←0;END ELSE BEGIN K1←1;K2←40;END;DA←DA1 FOR K←KK STEP K1         QEXP0160 SC  10;  1412
UNTIL K2 DO BEGIN DA1←ABS(AA[K]-A0);IF DA              TO INTERP ELSE BEG       QEXP0170 SC  10;  2411
IN DA←DA1;KK←K;END;END;WRITE(GEIL,                                                       SC  10;  2712
                          F1,A0); INTERP:COMMENT NOW USE LAGRANGE 3-PO          QEXP0180 SC  10;  3412
INT INTERPOLATION ;K1←KK-1;K2←KK+1;DA←AA[KK]-AA[K1];DA1←AA[K2]-AA[KK];C1        QEXP0190 SC  10;  6110
←(A0-AA[KK])×(A0-AA[K2])/(DA×(DA+DA1));C2←-(A0-AA[K1])×(A0-AA[K2])/(DA×D        QEXP0200 SC  10;  6710
A1);C3←(A0-AA[K1])×(A0-AA[KK])/((DA+DA1)×DA1);A0←3.141592×A0×A0×RHO×RHO         QEXP0210 SC  10;  5410
;Q[2,2,I,J]←(A0×(C1×I22[K1]+C2×I22[KK]+C3×I22[K2]))×2;END QEXP ;                QEXP0220 SC  10;  6111
                                                                   0019 IS 0077 LONG, NEXT SEG 0002
PROCEDURE COUL(T,N,Z1,Z2,B1,I,J);COMMENT    VERSION 9/25/65 ;COMMENT DEBY       COUL0010 SC   2;  1012
E,RST, ELEC, AND LAMBDA ARE GLOBAL VARIABLES AND MUST BE           DECLA        COUL0020 SC   2;  1012
RED PRIOR TO COUL ;VALUE T,N,Z1,Z2,B1,I,J;BOOLEAN B1;INTEGER I,J;REAL T,        COUL0030 SC   2;  1012
N,Z1,Z2;BEGIN REAL R0,INTER,LMBDA,PSI0;LABEL L1,L2;FORMAT F1(/10("*"),"T        COUL0040 SC   2;  1012
                                                                   START OF SEGMENT ........... 0023
                                                                   START OF SEGMENT ........... 0024
HE FOLLOWING PROPERTIES EVALUATED WITHOUT HIGHER ORDER TERMS IN CHARGED         COUL0050 SC  24;   81C
CROSS SECTIONS");  R0←5.35402@-4×Z1×Z2/T;INTER←1/(N×(T/3));DEBYE←SQRT(23        COUL0060 SC  24;   81C
                                                                   0024 IS 0022 LONG, NEXT SEG 0023
.81105×T/N));                  LMBDA←DEBYE/R0 ;                     PSI0←       COUL0070 SC  23;   611
LN(2×LMBDA);IF Z1<1.1AND Z2<1.1THEN BEGIN RST←PSI0;LAMBDA←LMBDA;ELEC←INT        COUL0080 SC  23;   912
ER;END;PSI0←2×PSI0;R0←R0×R0;IF NOT B1 THEN BEGIN          IF I=J THEN G         COUL0090 SC  23;  1810
O TO L1;Q[1,1,I,J]←3.14159×R0×R0×PSI0;Q[1,2,I,J]←Q[1,1,I,J]×2/3;Q[1,3,I,J]      COUL0100 SC  23;  2010
←.5×Q[1,2,I,J];Q[1,4,I,J]←.1×Q[1,1,I,J];Q[1,5,I,J]←.2×Q[1,2,I,J];Q[3,3,I        COUL0110 SC  23;  3411
,J]←.5×Q[1,1,I,J];L1:Q[2,2,I,J]←3.14159×R0×R0×PSI0;Q[2,3,I,J]←.5×Q[2,2,I        COUL0120 SC  23;  531C
,J];Q[2,4,I,J]←.3×Q[2,2,I,J];END ELSE BEGIN PSI0←PSI0-2.3099;R0←3.14159×        COUL0130 SC  23;  4712
R0×R0;IF I=J THEN GO TO L2;Q[1,1,I,J]←R0×(PSI0-1);Q[1,2,I,J]←R0×(PSI0-1)        COUL0140 SC  23;  4712
/3;Q[1,3,I,J]←R0×(PSI0-2)/4;Q[1,4,I,J]←R0×(PSI0-2.6667)×.1;Q[1,5,I,J]←R0        COUL0150 SC  23;  3811
×(PSI0-3.6667)/15;Q[3,3,I,J]←R0×(PSI0-.6667)×.5;L2:Q[2,2,I,J]←R0×PSI0;Q[        COUL0160 SC  23; 11212
2,3,I,J]←R0×(PSI0-1)×.5;Q[2,4,I,J]←R0×(PSI0-2.6667)×.3;END;END COUL ;           COUL0170 SC  23; 12410
PROCEDURE QCHX(A,B,M,I,T,J);COMMENT VERSION 9/28/65 ;VALUE A,B,M,T,I,J;R          0010 SC  23; 13410
                                                                   0023 IS 0147 LONG, NEXT SEG 0002
EAL A,B,M,T;INTEGER I,J;BEGIN COMMENT THIS PROCEDURE COMPUTES THE CHG TR          0020 SC   2;  1012
ANSFER CROSS SECTIONS WHEN     THE TOTAL CROSS SECTION IS FITTED TO THE F         0030 SC   2;  1012
UNCTION .5×(A-B.LN(G))↑2,      G = RELATIVE SPEED, UNITS ARE 10↑-16 CM↑2          0040 SC   2;  1012
;REAL X1,X2,LNTM,B2;LNTM←LN(T/(6.02252@23×M));B2←B×B;X2←(10.619×B2-2×A×B          0050 SC   2;  1012
                                                                   START OF SEGMENT ........... 0028
);X1←2×(A×A-19.619×A×B+96.226×B2)+LNTM×(X2+.5×B2×LNTM);Q[1,1,I,J]←.5×(X1          0060 SC  25;   51C
+.823×X2+B2×(.823+.923×LNTM));Q[1,2,I,J]←.5×(X1+1.256×X2+B2×(.931+1.256×          0070 SC  25;  141C
LNTM));Q[1,3,I,J]←.5×(X1+1.506×X2+B2×(1.285+1.506×LNTM));END QCHX ;               0080 SC  25;   51C
```

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                                                                    0025 IS 00A8 LONG, NEXT SEG 0002
PROCEDURE DETERM(NR,NC,N,E,DET,POW);COMMENT   VERSION 10/19/65 ;VALUE NR          0010 SC   2:  1912
,NC,N;INTEGER NC,NR,N,POW;REAL DET;REAL ARRAY E[0,0];BEGIN COMMENT NC AN          0020 SC   2:  1912
D NR ARE INDICES OF FIRST ROW AND FIRST COLUMN IN ARRAY OF WHICH THE DET          0030 SC   2:  1912
ERMINANT IS TO BE EVALUATED, N+1 IS RANK ;INTEGER J,K,P,Q,IND;REAL ARRAY          0040 SC   2:  1912
                                                                    START OF SEGMENT ********** 0026
 D[0:N,0:N];LABEL L1,L2;REAL FAC,ABSFAC,COLMAX,TEMP;FOR J←0STEP 1UNTIL N          0050 SC  26:   010
 DO FOR K←0STEP 1UNTIL N DO D[J,K]←E[J+NR,K+NC];POW←0;FAC←1;FOR J←0STEP          0060 SC  26:   410
1UNTIL N-1DO BEGIN COLMAX←ABS(D[J,J]);IND←J;FOR K←J+1STEP 1UNTIL N DO BE          0070 SC  26:  1611
GIN TEMP←ABS(D[K,J]);IF COLMAX<TEMP THEN BEGIN IND←K;COLMAX←TEMP;END;END          0080 SC  26:  2712
;FAC←D[IND,J]×FAC;IF FAC=0THEN GO TO L2;ABSFAC←ABS(FAC);FOR POW←POW+10WH          0090 SC  26:  3211
ILE ABSFAC>@1000 BEGIN FAC←@-10×FAC;ABSFAC←ABS(FAC);END;FOR POW←POW-10WH          0100 SC  26:  3613
ILE ABSFAC<@-1000 BEGIN FAC←@10×FAC;ABSFAC←ABS(FAC);END;IF IND=J THEN GO          0110 SC  26:  4712
 TO L1 ELSE FOR P←J STEP 1UNTIL N DO BEGIN TEMP←D[J,P];D[J,P]←D[IND,P];D          0120 SC  26:  5513
[IND,P]←TEMP;END;FAC←-FAC;L1:ABSFAC←1/D[J,J];FOR Q←J+1STEP 1UNTIL N DO D          0130 SC  26:  6113
[J,Q]←D[J,Q]×ABSFAC;D[J,J]←1;FOR P←J+1STEP 1UNTIL N DO BEGIN TEMP←D[P,J]          0140 SC  26:  7312
;FOR Q←J STEP 1UNTIL N DO D[P,Q]←D[P,Q]-D[J,Q]×TEMP;END;END;L2:DET←FAC×D          0150 SC  26:  8412
[N,N];END DETERM ;                                                                0160 SC  26:  9612
                                                                    0026 IS 0105 LONG, NEXT SEG 0002
PROCEDURE TRANS( T,P,N,  MAX,    SIGMA,LMBDA ) ;                            MEST0002 SC   2:  1912
 COMMENT T IN DEGREES K, P IN TORR, N IS ARRAY OF NUMBER DENSITIES: 0 =     MEST0003 SC   2:  1912
 ELECTRON, 1 = ATOM, 2 AND HIGHER = IONS, MAX IS INTEGER NUMBER OF SPECI    MEST0004 SC   2:  1912
 ES - 1, SIGMA AND LMBDA ARE ELECT AND THERMAL CONDUCTIVITIES ;             MEST0005 SC   2:  1912
 VALUE T,P,MAX ;                        REAL ARRAY   N[0] ;                 MEST0006 SC   2:  1912
 REAL T,P,SIGMA,LMBDA ;                 INTEGER MAX ;                       MEST0007 SC   2:  1912
 BEGIN                                                                      MEST0008 SC   2:  1912
    REAL ARRAY A[0:5,0:15],DIF[0:5] ;                                       MEST0009 SC   2:  1912
                                                                    START OF SEGMENT ********** 0027
    INTEGER I,J,L,K,K2,EXN,EXD,H ;                                          MEST0010 SC  27:   313
    LABEL L1 ;                                                              MEST0011 SC  27:   313
    REAL ION ;   COMMENT IONIZATION POTENTIAL IN DEGREES K ;                MEST0012 SC  27:   313
    REAL TROOT,TSQ,NTOT,RHO,LMDAA,LMDAE, ML2,NUM,DENOM,NMAX,   TM1,MI2,     MEST0013 SC  27:   313
       ML4,         LMDAR,DELH ;                                            MEST0014 SC  27:   313
    OWN REAL AC,BC,RHOA,RHOI,RHIOA,RHIOI,MN,MNSQR,TM3 ;                     MEST0015 SC  27:   313
    OWN REAL ARRAY M[0:5],MRT[0:5,0:5] ;    OWN BOOLEAN HIER ;              MEST0016 SC  27:   313
    DEFINE  FI1M = FOR I ← 1 STEP 1 UNTIL MAX DO #,                         MEST0017 SC  27:   813
            FJ1M = FOR J ← 1 STEP 1 UNTIL MAX DO #,                         MEST0018 SC  27:   813
            FL1M = FOR L ← 1 STEP 1 UNTIL MAX DO #,                         MEST0019 SC  27:   813
            FJIM = FOR J ← I+1 STEP 1 UNTIL MAX DO #,                       MEST0020 SC  27:   813
            FI0M = FOR I ← 0 STEP 1 UNTIL MAX DO #,                         MEST0021 SC  27:   813
            FJ0M = FOR J ← 0 STEP 1 UNTIL MAX DO # ;                        MEST0022 SC  27:   813
    LIST  T1( RHIOA,RHOA,RHIOI,RHOI,AC,BC, HIER, FI0M N[I] ) ;              MEST0023 SC  27:   813
    FORMAT FCROSS ( /"CROSS SECTIONS..."/ (9(F11.4,X1))),                   MEST0024 SC  27:  2812
                                                                    START OF SEGMENT ********** 0028
       FTHERM(/ "THERMAL CONDUCTIVY CONTRIBUTIONS AT T = ",F7.0," ARE:",    MEST0025 SC  28:  2812


         /"HEAVY ="E12.5," ELECTRON ="E12.5," REACTIVE ="E12.5,             MEST0026 SC  28:  2812
          " TOTAL ="F12.5 ) ;                                               MEST0027 SC  28:  2812
                                                                    0028 IS 00A1 LONG, NEXT SEG 0027
    IF AC = 0 THEN BEGIN                                                    MEST0028 SC  27:  2812
READ(READER,/,T1);                                                                   SC  27:  2913
       FI1M                                                                 MEST0030 SC  27:  3311
          M[I] ← M[I] / 6.02252@23 ;                                        MEST0031 SC  27:  3410
       TM3 ← 1.38054@-46 / M[0] / M[0] / M[0] ;                             MEST0032 SC  27:  3811
       MN ← M[1] ;                                                          MEST0033 SC  27:  4111
       MNSQR ← SQRT(MN) ;                                                   MEST0034 SC  27:  4211
       FI0M    BEGIN                                                        MEST0035 SC  27:  4312
          M[I] ← M[I] / MN ;                                                MEST0036 SC  27:  4710
          MRT[I,I] ← SQRT(M[I]) ;    END ;                                  MEST0037 SC  27:  4910
       FI0M    FJIM                                                         MEST0038 SC  27:  5410
          MRT[I,J] ←MRT[J,I] ← SQRT(M[I] + M[J]) ;                          MEST0039 SC  27:  5011
       END ;                                                                MEST0040 SC  27:  6711
    TROOT ← SQRT(T) ;    TSQ ← T×T ;    NTOT ← RHO ← 0 ;                    MEST0041 SC  27:  6711
    FI0M    BEGIN                                                           MEST0042 SC  27:  7110
       NTOT ← NTOT + N[I] ;                                                 MEST0043 SC  27:  7210
       RHO ← RHO + N[I]×M[I] ; END ;                                        MEST0044 SC  27:  7312
    RHO ← RHO × MN ;                                                        MEST0045 SC  27:  7810
    QEXP( RHIOA,RHOA,T,1,1 ) ;                                              MEST0046 SC  27:  7911
       LMDAA ← 3.34028@-8×TROOT/(MNSQR×Q[2,2,1,1]) ;                        MEST0047 SC  27:  8110
    COUL( T,N[0],1,1,HIER, 0,2 ) ;                                          MEST0048 SC  27:  8513
    Q[2,2,2,2]  ← Q[2,2,0,2] ;                                              MEST0049 SC  27:  8811
    FOR J ← 2,3,4 DO                                                        MEST0050 SC  27:  9411
       Q[2,J,0,0] ← Q[2,J,0,2] ;                                            MEST0051 SC  27: 10013
    QFXE( T,0,1 ) ;                                                         MEST0052 SC  27: 10910
    Q[2,2,1,2] ← Q[2,2,1,1] ;                                               MEST0053 SC  27: 11011
    QCHX(AC,BC,MN  ,T,1,2 ) ;                                               MEST0054 SC  27: 11611
    FI1M                                                                    MEST0055 SC  27: 11811
       FJIM                                                                 MEST0056 SC  27: 11910
          FOR K ← 1,2 DO    BEGIN                                           MEST0057 SC  27: 12311
             IF K = 1 THEN K2 ← 3 ELSE K2 ← 2 ;                             MEST0058 SC  27: 12713
             FOR L ← K STEP 1 UNTIL K2 DO                                   MEST0059 SC  27: 13110
                Q[K,L,J,I] ← Q[K,L,I,J] ;  END ;                            MEST0060 SC  27: 13210
    FI1M                                                                    MEST0061 SC  27: 14312
          FOR K ← 1 STEP 1 UNTIL 3 DO BEGIN                                 MEST0062 SC  27: 14510
             IF K = 1 THEN K2 ← 5 ELSE                                      MEST0063 SC  27: 14610
             IF K = 2 THEN K2 ←4                                            MEST0064 SC  27: 14810
             ELSE K2 ← 3 ;                                                  MEST0065 SC  27: 14913
             FOR L ← K STEP 1 UNTIL K2 DO                                   MEST0066 SC  27: 15113
                Q[K,L,I,0] ← Q[K,L,0,I] ;  END ;                            MEST0067 SC  27: 15310
    DIF[I] ←              7.80968@7×TROOT×SQRT(1/MN)/(NTOT×Q[1,1,1,2]) ;    MEST0068 SC  27: 16513
    L ← 3 × (MAX + 1) ;                                                     MEST0069 SC  27: 17212
```

```
FOR I ← 0 STEP 1 UNTIL L DO
   FOR J ← I STEP 1 UNTIL L DO
      A[I,J] ← A[J,I] ← 0 ;
NMAX ← N[0] ;
FLIM
   IF N[I] > NMAX THEN NMAX ← N[I] ;
FIOM
   N[I] ← N[I] / NMAX ;
FJIM            COMMENT  Q00IJ ;
   BEGIN
   FLIM
      A[0,J] ← A[0,J] + N[L] × Q[1,1,0,L] ;
   A[0,J] ← -8 × N[J] × MRT[J,J] × A[0,J] / MRT[0,0] ;
   END ;
FJIM            COMMENT  Q00J1 ;
   BEGIN
   FLIM
      IF L ≠ J THEN A[J,0] ← A[J,0] + N[L] × (MRT[L,L]/MRT[J,L]) ×
      Q[1,1,J,L] ;
   A[J,0] ← -8 × N[0] × (N[J] × Q[1,1,0,J] + A[J,0] × (MRT[0,0] /
      MRT[J,J]) ) ;
   END ;
FIIM            COMMENT  Q00IJ ;
   FJIM
      IF I ≠ J THEN  BEGIN
         FLIM
            IF I ≠ L THEN  A[I,J] ← A[I,J] + N[L] × MRT[L,I] ×
               MRT[J,J]×Q[1,1,I,L]/(MRT[I,I] × MRT[I,L]) ;
      A[I,J] ← -8 × N[J] × (A[I,J] + N[I] × MRT[1,I] × Q[1,1,I,J]
               / MRT[I,J]);   END ;
K ← MAX + 1 ;
FLIM            COMMENT  Q01I1 ;
   A[0,K] ← A[0,K] + N[L] × (2.5 × Q[1,1,0,L] - 3 × Q[1,2,0,L]) ;
A[0,K] ← 8 × N[0] × A[0,K] ;
FIIM  BEGIN     COMMENT  Q01II ;
   FLIM
      IF L ≠ I THEN A[I,K+I] ← A[I,K+I] + N[L] ×(MRT[L,L]/MRT[I,L])+
         3 × (2.5 × Q[1,1,I,L] - 3 × Q[1,2,I,L]) ;
   A[I,K+I] ← 8 × N[I] × A[I,K+I] ;
   END ;
FJIM  BEGIN     COMMENT  Q01J1,Q01IJ ;
   A[J,K] ← - 8 × N[0] × N[J] × (2.5 × Q[1,1,0,J] - 3 × Q[1,2,0,J]);
   A[0,J+K] ← A[J,K] ×(MRT[0,0] / MRT[J,J])+3 ;
      END ;
FIIM            COMMENT  Q01IJ ;



   FJIM
      BEGIN
      A[I,J+K] ← -8 × N[I] × N[J] × (MRT[1,I]/MRT[I,J])+3 ×
               (2.5 × Q[1,1,I,J] - 3 × Q[1,2,I,J]) ;
      A[J,I+K] ← A[I,J+K] × (MRT[J,J] / MRT[I,I])+3 ;
      END ;
FIOM            COMMENT  Q10IJ ;
   FJOM
      A[I+K,J] ← (M[J]/M[I]) × A[I,J+K] ;
FLIM            COMMENT  Q1111 ;
   A[K,K] ← A[K,K] + N[L] × (6.25 × Q[1,1,0,L] - 15 × Q[1,2,0,L]
         + 12 × Q[1,3,0,L]);
A[K,K] ← 8 × N[0] × (A[K,K] + 1.AIA21 × N[0] × Q[2,2,0,0] ) ;
FJIM            COMMENT Q111J,Q11J1 ;
   BEGIN
   A[K,K+J] ← -8 × N[0] × N[J] × (MRT[0,0]/MRT[J,J])+3 × (13.75 ×
   Q[1,1,0,J]-15×Q[1,2,0,J]+12×Q[1,3,0,J] - 4 × Q[2,2,0,J]) ;
   A[K+J,K] ← A[K,K+J] × MRT[J,J]/MRT[0,0] ;
   END ;
FIIM            COMMENT  Q11II ;
   BEGIN
   FLIM
      IF L ≠ I THEN
         BEGIN
         ML2 ← M[L]+2 ;
         A[K+I,K+I] ← A[K+I,K+I] + N[L] × MRT[L,L]×(1.25 ×(8×M[I]+2
         + 5×ML2)×Q[1,1,I,L] - 15×ML2×Q[1,2,I,L] + 12×ML2×Q[1,3,I,L]
         + 8×M[I]×M[L]×Q[2,2,I,L]) / MRT[I,L]+5 ;
      END ;
   A[K+I,K+I] ← 8 × N[I] × (A[K+I,K+I] + 1.AIA21A×N[I]×Q[2,2,1,1]);
   END ;
FIIM            COMMENT  Q11IJ ;
   FJIM
      BEGIN           A[K+I,K+J] ← -8 × N[I] × N[J] × M[J] × MRT[1,I]
         +3 × (13.75×Q[1,1,I,J] - 15 × Q[1,2,I,J] + 12 × Q[1,3,I,J]
         -4 × Q[2,2,I,J]) / MRT[I,J]+5 ;
      A[K+J,K+I] ← MRT[J,J] × A[K+I,K+J] / MRT[I,I] ;
      END ;
COMMENT COMPUTE HEAVY CONTRIBUTION TO THERMAL CONDUCTIVITY ;
K2 ← K ;
K ← 2 × K ;
TM1 ← - 3.8118A8-7 × TROOT / MNSQR ;
FIIM
   A[K,K2+I] ← N[I] / MRT[1,I] ;
FIOM
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      A[K2+I,K] ← N[I] ;                                          WEST0140 SC  27:
   DETERM( K2+1,K2+1,K2-1,A,NUM,EXN ) ;                            WEST0141 SC  27:
   DETERM( K2+1,K2+1,K2-2,A,DENOM,EXD ) ;                          WEST0142 SC  27:
   LMDAA ← TM1 × NUM × 10*(EXN-EXD) / DENOM ;                      WEST0143 SC  27:
   L ← 3 × (MAX + 1) ;                                             WEST0144 SC  27:
   A[L,M2] ← 1 ;                                                   WEST0145 SC  27:
   FIOM                                                            WEST0146 SC  27:
      BEGIN                                                        WEST0147 SC  27:
      A[K2+I,L] ← A(K2+I,K] ;                                      WEST0148 SC  27:
      A[K2+1,K] ← 0 ;                                              WEST0149 SC  27:
      END ;                                                        WEST0170 SC  27:
   FI1M                                                            WEST0171 SC  27:
      A[K,K2+I] ← 0 ;                                              WEST0172 SC  27:
BEGIN    INTEGER NEWBLOCK ;                                        WEST0173 SC  27:
                                              START OF SEGMENT ********** 0025
                                                                   WEST0174 SC  20:
   FL1M              COMMENT  Q1211 ;                              WEST0175 SC  20:
      A[K2,K] ← A[K2,K] + N[L] × (10,0375×Q[1,1,0,L] -39,375×Q[1,2,0,L]   WEST0176 SC  20:
         + 57×Q[1,3,0,L] - 30×Q[1,4,0,L]) ;                        WEST0177 SC  20:
   A(K2,K] ← N[0] × (1,414214×N(0]×(16×Q[2,2,0,0] - 16×Q[2,3,0,0])  WEST0178 SC  20:
           + R × A[K2,K]] ;                                        WEST0179 SC  20:
   FI1M              COMMENT  Q1211 ;                              WEST0180 SC  20:
      BEGIN                                                        WEST0181 SC  20:
      J ← K + I ;     H ← K2 + 1 ;                                 WEST0182 SC  20:
      MI2 ← M[I] × M[I] ;                                          WEST0183 SC  20:
      FL1M                                                         WEST0184 SC  20:
         BEGIN                                                     WEST0185 SC  20:
         ML2 ← M[L] × M[L] ;                                       WEST0186 SC  20:
         IF L ≠ I THEN                                             WEST0187 SC  20:
         A[H,J] ← A[H,J] + N[L] ×(WRT[L,L]*3/WRT[I,L]*7) × (2,187K×   WEST0188 SC  20:
            (12×MI2 + 5×ML2)×Q[1,1,I,L] - 31,5×(MI2 + 1,2×ML2)×      WEST0189 SC  20:
            Q[1,2,I,L] + 57×ML2×Q[1,3,I,L] - 30×ML2×Q[1,4,I,L] +      WEST0190 SC  20:
            18×M[I]×M[L]×Q[2,2,I,L] - 16×M[I]×M[L]×Q[2,3,I,L]) ;      WEST0191 SC  20:
         END ;                                                     WEST0192 SC  20:
      A[H,J] ← N[I] × (1,414214 N[I]×(16×Q[2,2,I,I] - 16×Q[2,3,I,I])   WEST0193 SC  20:
            + R × A[H,J]) ;                                        WEST0194 SC  20:
      END ;                                                        WEST0195 SC  20:
   FJ1M              COMMENT  Q121J,Q12J1 ;                        WEST0196 SC  20:
      BEGIN                                                        WEST0197 SC  20:
      A[K2,K+J]←   N[0]×N[J]×(WRT[0,0]/WRT[J,J])*5×(37,1875×Q[1,1,0,J]   WEST0198 SC  20:
         - 70,875 ×Q[1,2,0,J] + 57×Q[1,3,0,J] - 30×Q[1,4,0,J]      WEST0199 SC  20:
         - 16×Q[2,2,0,J] + 16×Q[2,3,0,J]) ;                        WEST0200 SC  20:
      A[K2+J,K] ← (WRT[J,J]/WRT[0,0])*3 × A[K2,K+J] ;              WEST0201 SC  20:
      END ;                                                        WEST0202 SC  20:
   FI1M              COMMENT  Q121J ;                              WEST0203 SC  20:
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      FJIM                                                         WEST0204 SC  20:
         BEGIN                                                     WEST0205 SC  20:
         A[K2+I,K+J] ← +R × N[I] × N[J] ×(WRT[I,I]*5×M[J]/WRT[I,J]*7) ×   WEST0206 SC  20:
            (37,1875×Q[1,1,I,J] - 70,875×Q[1,2,I,J] + 57×Q[1,3,I,J] -    WEST0207 SC  20:
            30×Q[1,4,I,J] - 16×Q[2,2,I,J] + 16×Q[2,3,I,J]) ;       WEST0208 SC  20:
         A[K2+J,K+I] ← (WRT[J,J]/WRT[I,I])*3 × A[K2+I,K+J] ;       WEST0209 SC  20:
         END ;                                                     WEST0210 SC  20:
   FI0M              COMMENT  Q211J ;                              WEST0211 SC  20:
      FJ0M                                                         WEST0212 SC  20:
         IF I = J THEN A[K+I,K2+J] ← A[K2+I,K+J]                   WEST0213 SC  20:
         ELSE A[K+I,K2+J]← (M[J]/M[I]) × A[K2+I,K+J] ;             WEST0214 SC  20:
   FL1M              COMMENT  Q2211 ;                              WEST0215 SC  20:
      A[K,K] ← A(K,K] + N[L] × (10,140625×Q[1,1,0,L] -91,875×Q[1,2,0,L]   WEST0216 SC  20:
         + 199,5×Q[1,3,0,L] - 210×Q[1,4,0,L] + 90×Q[1,5,0,L]) ;    WEST0217 SC  20:
   A[K,K] ← N[0] × ( ,7071067×N(0]×(77×Q[2,2,0,0] - 112×Q[2,3,0,0] +   WEST0218 SC  20:
      80×Q[2,4,0,0]) + R × A[K,K]] ;                               WEST0219 SC  20:
   FI1M              COMMENT  Q22II ;                              WEST0220 SC  20:
      BEGIN                                                        WEST0221 SC  20:
      MI2 ← M[I] × M[I] ;                                          WEST0222 SC  20:
      J ← K + I ;                                                  WEST0223 SC  20:
      FL1M                                                         WEST0224 SC  20:
         BEGIN                                                     WEST0225 SC  20:
         ML2 ← M[L] × M[L] ;                                       WEST0226 SC  20:
         ML4 ← ML2 × ML2 ;                                         WEST0227 SC  20:
         IF L ≠ I THEN                                             WEST0228 SC  20:
         A[J,J] ← A[J,J] + N[L] ×(WRT[L,L]/WRT[I,L]*9) × (,8448?5×    WEST0229 SC  20:
            (40×MI2×MI2 + 168×MI2×ML2 + 35×ML4)×Q[1,1,I,L]-ML2×(2,425×   WEST0230 SC  20:
            (84×MI2 +35×ML2)×Q[1,2,I,L] - 1,5×    (10×MI2+ 13×ML2)×      WEST0231 SC  20:
            Q[1,3,I,L])-ML4×(210×Q[1,4,I,L] - 90×    Q[1,5,I,L])+        WEST0232 SC  20:
            2×M[I]×M[L]×(4×MI2 +7×ML2)×Q[2,2,I,L] - M[I]×M[L]×ML2×      WEST0233 SC  20:
            (112×Q[2,3,I,L] - 80×Q[2,4,I,L]) + 24×MI2×ML2×Q[3,3,I,L]) ; WEST0234 SC  20:
         END ;                                                     WEST0235 SC  20:
      A[J,J] ← N[I] × (,7071067×N[I]×(77×Q[2,2,I,I] - 112×Q[2,3,I,I]   WEST0236 SC  20:
         + 80×Q[2,4,I,I]) + R × A[J,J]) ;                          WEST0237 SC  20:
      END ;                                                        WEST0238 SC  20:
   FJ1M              COMMENT  Q221J,Q22J1 ;                        WEST0239 SC  20:
      BEGIN                                                        WEST0240 SC  20:
      A[K,K+J] ← -R×(WRT[0,0]/WRT[J,J])*5 ×(142,890625×Q[1,1,0,J] -   WEST0241 SC  20:
         312,375×Q[1,2,0,J] +-341,5×Q[1,3,0,J] - 210×Q[1,4,0,J] +    WEST0242 SC  20:
         90×Q[1,5,0,J] - 77×Q[2,2,0,J] + 112×Q[2,3,0,J] - 80×Q[2,4,0,J]  WEST0243 SC  20:
         + 24×Q[3,3,0,J]) × N[0] × N[J] ;                          WEST0244 SC  20:
      A[K+J,K] ← (WRT[J,J]/WRT[0,0]] × A[K,K+J] ;                  WEST0245 SC  20:
      END ;                                                        WEST0246 SC  20:
   FI1M              COMMENT  Q22IJ ;                              WEST0247 SC  20:
      FJIM                                                         WEST0248 SC  20:
```

```
        BEGIN                                                                   WEST0249 SC  20: A1A11
        A[K+I,K+J] ← -8×N[I]×N[J]×(MRT[I,I]+5×M[J]*2/MRT[I,J]*9) ×              WEST0250 SC  20: A1A11
           (132.890625×Q[1,1,I,J] - 312.375×Q[1,2,I,J] + 361.5×                 WEST0251 SC  20: A2A11
           Q[1,3,I,J] - 210×Q[1,4,I,J] + 90×Q[1,5,I,J] - 77×Q[2,2,I,J]          WEST0252 SC  20: A3311
           +112×Q[2,3,I,J] - 80×Q[2,4,I,J] + 24×Q[3,3,I,J]) ;                   WEST0253 SC  20: A4A1C
        A[K+J,K+I] ← MRT[J,J]×A[K+I,K+J]/MRT[I,I] ;                             WEST0254 SC  20: A5A11
        END ;                                                                   WEST0255 SC  20: A6A11
   COMMENT COMPUTE ELECTRON THERM. COND ;                                       WEST0256 SC  20: A7211
   DETERM(K2,K2,K-1,A,DENOM,EXD) ;                                              WEST0257 SC  20, A7211
   DETERM(K2,K2,K,A,NUM,EXN) ;                                                  WEST0258 SC  20: A7512
   LMDAE ← TM1 × NUM × 10*(EXN - EXD) × N[0] / (DENOM × MRT[0,0]) ;             WEST0259 SC  20: A7811
   K ← 3 × (MAX + 1) ;                                                          WEST0260 SC  20: A8511
   A[K,K2] ← 0 ;                                                                WEST0261 SC  20: A871C
   FIOM                                                                         WEST0262 SC  20: A891C
      A[K2+I,K] ← 0 ;                                                           WEST0263 SC  20: A901C
   K ← 2 × (MAX + 1) ;                                                          WEST0264 SC  20: A9413
   FLIM              COMMENT  Q0211 ;                                           WEST0265 SC  20: A9A12
      A[0,K] ← A[0,K] + N[L] × (4.375×Q[1,1,0,L] - 10.5×Q[1,2,0,L]              WEST0266 SC  20: A981C
              + 6×Q[1,3,0,L]) ;                                                 WEST0267 SC  20: A971C
   A[0,K] ←   8 × N[0] × A[0,K] ;                                               WEST0268 SC  20: 51A12
   FIIM              COMMENT  Q021I ;                                           WEST0269 SC  20: 51813
      BEGIN                                                                     WEST0270 SC  20: 5221C
      J ← K+I ;                                                                 WEST027  SC  20: 5221C
      FLIM                                                                      WEST0272 SC  20: 52311
         IF L ≠ I THEN A[I,J] ← A[I,J] + N[L]×(MRT[L,L]/MRT[I,L])*5 ×           WEST0273 SC  20: 5261C
            (4.375×Q[1,I,I,L] - 10.5×Q[1,2,I,L] + 6×Q[1,3,I,L]) ;               WEST0274 SC  20: 53213
      A[I,J] ←  8 × N[I] × A[I,J] ;                                             WEST0275 SC  20: 56A11
      END ;                                                                     WEST0276 SC  20: 58012
   FJIM              COMMENT  Q02J1,Q021J ;                                     WEST0277 SC  20: 55213
      BEGIN                                                                     WEST0278 SC  20: 55A1C
      A[J,K] ← -8 × N[0] × N[J] × (4.375×Q[1,1,0,J] - 10.5×Q[1,2,0,J]           WEST0279 SC  20: 55A1C
              + 6×Q[1,3,0,J]) ;                                                 WEST0280 SC  20: 56A11
      A[0,K+J] ← (MRT[0,0]/MRT[J,J])*5 × A[J,K] ;                               WEST0281 SC  20: 57011
      END ;                                                                     WEST0282 SC  20: 57811
   FIIM              COMMENT  Q02IJ ;                                           WEST0283 SC  20: 58012
      FJIM                                                                      WEST0284 SC  20: 5841C
         BEGIN                                                                  WEST0285 SC  20: 58811
         A[I,K+J] ← -8 × N[I] × N[J]×(MRT[I,I]/MRT[I,J])*5 × (4.375 ×           WEST0286 SC  20: 58811
            Q[1,1,I,J] - 10.5×Q[1,2,I,J] + 6×Q[1,3,I,J]) ;                      WEST0287 SC  20: 59413
         A[J,K+I]←(MRT[J,J]/MRT[I,I])*5 × A[I,K+J] ;                            WEST0288 SC  20: A0712
         END ;                                                                  WEST0289 SC  20: A1A1C
   FIOM              COMMENT  Q20IJ ;                                           WEST0290 SC  20: A2111
      FJOM                                                                      WEST0291 SC  20: A221C
         IF I = J THEN A[K+I,J] ←  A[I,K+J]                                     WEST0292 SC  20: A231C
         ELSE A[K+I,J] ← (M[J]/M[I])*2 × A[I,K+J] ;                             WEST0293 SC  20: A2712


   K ← 3×(MAX+1) ;                                                              WEST0294 SC  20: A3011
   COMMENT  NOW COMPUTE 3RD APPROX TO ELECT COND ;                              WEST0295 SC  20: A311C
   TM1 ← 4.4177088 × RHO × TROOT / (MN × NMAX × NTOT × MNSQR) ;                 WEST0296 SC  20: A311C
   SIGMA ← 0 ;                                                                  WEST0297 SC  20: A4A11
   DETERM(0,0,K-1,A,DENOM,EXD ) ;                                               WEST0298 SC  20: A4511
   A[0,K] ← -1 ;                                                                WEST0299 SC  20: A491C
   FOR I ← 2 STEP 1 UNTIL MAX DO                                                WEST0300 SC  20: A5111
      BEGIN                                                                     WEST0301 SC  20: A531C
      A[I,K] ← 1 ;                                                              WEST0302 SC  20: A531C
      DETERM( 0,1,K-1,A,NUM,EXN) ;                                              WEST0303 SC  20: A5S1C
      DIFF[I]   ← TM1 × N[0] × NUM ×  10*(EXN - EXD)  / (M[I]×MRT[0,0]          WEST0304 SC  20: A5811
         × DENOM) ;                                                             WEST0305 SC  20: A6413
      SIGMA ← SIGMA + N[I] × M[I] × (I-1) × DIFF[I] ;                           WEST0306 SC  20: A6A12
      A[I,K] ← 0 ;                                                              WEST0307 SC  20: A7013
      END ;                                                                     WEST0308 SC  20: A7213
   A[0,K] ← 0 ;                                                                 WEST0309 SC  20: A751C
   SIGMA ←-1.85678-15 × NTOT × NMAX × MN × SIGMA / (RHO × T) ;                  WEST0310 SC  20: A771C
   FIOM                                                                         WEST0311 SC  20: A8111
      N[I] ← NMAX × N[I] ;                                                      WEST0312 SC  20: A831C
   ION ← 27833.4 ;                                                              WEST0313 SC  20: A8713
   DELH ← 1.38054@-16 × (2.5 × T + ION) ;                                       WEST0314 SC  20: A881C
   LMDAR ← DELH × (N[0]×N[1]×NTOT/(1.38054@-16×T*2×(N[0]+N[1])*2) ×             WEST0315 SC  20: A9011
         DELH × DIFF[1]);                                                       WEST0316 SC  20: A9813
 END ;                                                                          WEST0317 SC  20: A9713
                                                              0020 IS 0702 LONG, NEXT SEG 0027
 L1:                                                                            WEST0318 SC  27: A081C
   LMBDA← LMDAA + LMDAE + LMDAR ;                                               WEST0319 SC  27: A081C
WRITE(GEIL,ETHERM,                                                                       SC  27: A101C
   T,THEAVY[IT]←LMDAA,TELEC[IT]←LMDAE,TREACT[IT]←LMDAR,TTOT[IT]←LMBDA);                  SC  27: A1212
 END TRANS ;                                                                    WEST0321 SC  27   311C
                                                              0027 IS 0483 LONG, NEXT SEG  02
READ(READER,/,NAM,MAX);                                                                  SC   21  101?
READ(READER,/,T1,DT,TMAX);                                                               SC   21  3013
READ(READER,/,NP,FOR I←1 STEP 1 UNTIL NP DO PR[I]);                                      SC   21  4313
WRITE(PUNCH,PUNCHA,T1,DT,TMAX);                                                          SC   21  6811
FOR IP←1 STEP 1 UNTIL NP DO BEGIN                                                        SC   21  7111
P←PR[IP]×760;                                                                            SC   21  721C
WRITE(GEIL [PAGE] ) ;                                                                    SC   21  7312
WRITE(GEIL,FP,NAM,P/760 ) ;                                                              SC   21  7411
WRITE(PUNCH,PUNCHA,P/760);                                                               SC   21  8011
IT←0;                                                                                    SC   21  10011
FOR T←T1 STEP DT UNTIL TMAX DO                                                           SC   21  1011C
      BEGIN                                                                              SC   21  1021C
TEMP[IT]←T/2000;                                                                         SC   21  1021C
      SAHA( T,P,ALF ) ;                                                                  SC   21  10313
```

```
            NTOT ← 9.6573018 × P / T ;                                          SC   21 10510
            N[0] ← N[2] ← ALF × NTOT /(1 + ALF) ;                               SC   21 10613
            N[1] ← NTOT × (1 - ALF) / (1 + ALF) ;                               SC   21 11012
            TRANSC( T,P,N,  MAX,     SIGMA[IT],LMBDA ) ;                        SC   21 11313
         WRITE(GFIL,FI,T, FOR I ← 0 STEP 1 UNTIL 2 DO [T,N[I]],N[0]/(N[0]+     SC   21 12011
                N[1]),DERYE,ELT(,LAMBDA,SIGMA[T] ,LMBDA ) ;                     SC   21 13513
      IT←IT+1;                                                                   SC   21 14711
      END;                                                                       SC   21 14812
      WRITE(GFIL).                                                               SC   21 15113
      WRITE(GFIL,CLOCK,TIME(2)/60,TIME(3)/60);                                  SC   21 15812
      IT←IT+1;                                                                   SC   21 16911
      END;                                                                       SC   21 17012
      CLOSEDECK(PUNCH,GFIL);                                                     SC   21 17213
      END.                                                                       SC   21 17411
                                                           0002 IS 0177 LONG, NEXT SEG 0002
    EXP              IS SEGMENT NUMBER 0030, PRT ADDRESS IS 011A
    LN                                 0031             0117
    SQRT                               0032             0121
    OUTPUT(W)                          0033             0052
    BLOCK CONTROL                      0034             0005
    INPUT(W)                           0035             0160
    X TO THE I                         0036             0120
    ALGOL WRITE                        0037             001A
    ALGOL READ                         0038             0015
    ALGOL SELECT                       0039             001A
NUMBER OF ERRORS DETECTED = 000                         LAST CARD WITH ERROR HAS SEQ #
PRT SIZE=0141;    TOTAL SEGMENT SIZE=02A12 WORDS;    DISK STORAGE REQ.=0301A WORDS;    NO. SEGS.=0040.
ESTIMATED CORE STORAGE REQUIREMENT = 0A97A WORDS.
20:23:08 FRIDAY, [illegible] [illegible], [illegible]    PROCESSOR TIME = 37.47 SECONDS    I/O TIME = 51.42 SECONDS
```

LABEL 000000000LINE   00166330?2 COMPILE ELEC/THERM LIBRARY   1E0828CC ALGOL

APPENDIX B

CALCULATION OF BOUND-BOUND TRANSITION PROBABILITIES

by D. Sun

The overall purpose of the system of programs being developed is to represent the spectrum of an atomic species in a plasma, including all lines and portions of the continuum which carry a significant portion of the energy. Hence it will be necessary to calculate large numbers of transition probabilities for bound-bound, bound-free, and free-free transitions.

Calculation of the bound-bound case to be discussed here is fairly complete; the other two types of transitions have not been added yet. The program to be described, presently called GIANT/FIASCO, consists of four sub-programs, (following the format of E. Corinaldesi) between which information is transferred by three disc files, READF1, READF2, and READF3. Programs 1 and 2 are run together, and accepting as their input the quantum numbers and energies of the various energy levels of a species as they are given in Moore's tables.[1] Program 2 prints out transition probabilities for all transitions allowed by the selection rules within the range considered. These are also placed on the disc READF2 where they may be tapped by Program 3 or by an auxillary program FIASCO/RESULTS, which merely prints out the results in a number of convenient forms. Program 3 calculates the Stark shift and broadening of each level, while Program 4 combines these into the shift and broadening of each spectral line. However, this paper is concerned primarily with Programs1 and 2, the calculation of bound-bound transition probabilities.

The heart of the matter is the calculation of $|\langle\psi_n|z|\psi_m\rangle|^2$ where ψ_n, and ψ_m are the two states between which a transition may occur

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[1] C. Moore, Atomic Energy Levels, National Bureau of Standards, Circular 467, U.S. Government Printing Office, Washington, D.C.

[2] E. Corinaldesi, to be published.

and $z=r\cos\theta$ is the electric dipole operator. (Quadrupole and magnetic dipole transitions are ignored.) Although ψ_n, ψ_m, and z actually involve all the electrons in the atom, in practice, it is possible to use the one-electron wave functions of the outer electron which makes the transition (Condon and Shortley, Section 6[3]).[3] Now each energy level consists of 2J+1 states with different z-components of angular momentum. For transitions from n to m, it is necessary to sum the square of the matrix element for all of the m-states, and average it over all of the initial n-states. The oscillator strength f_{nm} is $\frac{4\pi mc\bar{\nu}}{f_n}$ times this quantity, and the following relations hold:

$$(2J_n + 1)f_{nm} = gf = (2J_m + 1)f_{mn}$$

$$A_{nm} = 0.667 \times \bar{\nu}^2 \quad \text{where } \bar{\nu} \text{ is in cm}^{-1}$$

$$(2J_n + 1)A_{nm} = (2J_m + 1)A_{mn}$$

The solutions to Schroedinger's equation separate into two parts, giving the form $\frac{R(r)}{r} Y(\theta, \phi)$. R(r) is known as the radial wave function while $Y(\theta, \phi)$ is the angular part Hence the problem separates into a radial integral $\int_0^\infty R_n R_m dr$, and an averaging and summing process which is carried out using Racah coefficients of the quantum numbers of the initial and final states.

THE ANGULAR PART (COUPLING SCHEMES)

When an atom with more than one electron is being considered, there are several ways to add the multiple orbital and spin angular momentums. For example, one might add all the orbital angular momentum

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[3] E. Condon and G. Shortley, Theory of Atomic Spectra, Cambridge University Press, London (1935) hereafter referred to as Condon and Shortley and the Section.

operators to get a total orbital angular momentum operator, and do the same with the spin operators. Then the total orbital angular momentum operator and the total spin angular momentum operator might be added to give a total angular momentum. If the actual states of the atom closely approximate the eigenstates of the total orbital and spin angular momentum operators, then the atom is said to be LS coupled, the L and S representing good quantum numbers of the operators. One way to express the states is to put the quantum numbers of two operators in brackets to the left of the quantum number for the sum of the two operators. An LS state is written $|[S, (L_{core}, \ell)L]J\rangle$, where L_{core} is the total L of the inner electrons, ℓ is the orbital quantum number of the outer electron, and J is the total angular momentum. A form of coupling commonly found in the rare gases is jℓ coupling, given by $|[(J_{core}, \ell)K, S]J\rangle$, where J_{core} is the total angular momentum of the core, s is the spin of the outer electron, and K is the intermediate quantum number.

The average and sum over the initial and final states for $|\langle\psi_n|z|\psi_m\rangle|^2$ is easily seen to be equal to one third of the same average and sum for $|\langle\psi_n|\vec{r}|\psi\rangle|^2$. $\vec{r}$ turns out to be a class $\vec{T}$ operator with respect to J (See Condon and Shortley, 8^3). Here it is convenient to introduce a quantity $\langle j\|T\|j'\rangle$ which can be related to the components of the matrix element $\langle jm|\vec{T}|j'm'\rangle$ but is itself independent of m and m', the z-components. (See Condon and Shortley, 9^3). Now if $[P,J_1] = 0$ and P is class T with to $J = J_1 + J_2$, then the ratio

$$\frac{|\langle j_1 j_2 j\|P\|j_1 j_2' j'\rangle|^2}{|\langle j_1 j_2\|P\|j_1 j_2'\rangle|^2}$$

is given by Equation $11^3 8$ of Condon and Shortley, or by $(2j' + 1)j_{2>}(2j_2 + 1)(2j_2' + L)W^2(j_2,j,j_2',j';j_1)/\Xi(j,j')$ where $j_{2>} = \max(j_2,j_2')$, $W(j_2,j,j_2',j';j_1)$ is the Racah coefficient, and $\Xi(j,j')$ is defined by:

$$\Xi(j,j+1) = (j+1)(2j+3)$$

$$\Xi(j,j) = j(j+1)$$

$$\Xi(j,j-1) = j(2j-1) \qquad \text{See Condon and Shortley, } 7^4 5$$

In the program there are two procedures, XI and W2MOD, with XI(j,j') = $\Xi(j,j')$ and with W2MOD(j_2,j,j_2',j',j_1)/XI(j,j') equal to the above ratio.

Returning to LS and jl coupling, we have:

$$|\langle [S,(L_{core},\ell)L]J \vdots r \vdots [S,(L_{core},\ell')L']J' \rangle|^2 =$$

$$\frac{W2MOD(L,J,L',J',S)}{XI(J,J')} \; |\langle (L_{core},\ell)L \vdots r \vdots (L_{core},\ell') : ' \rangle|^2 =$$

$$\frac{W2MOD(L,J,L',J',S)\; W2MOD(\ell,L,\ell',L',L_{core})}{XI(J,J')\; XI(L,L')} \; |\langle \ell \vdots r \vdots \ell' \rangle|^2$$

for LS coupling, and

$$|\langle [(J_{core},\ell)K,s]J \vdots r \vdots [J_{core},\ell')K',s]J' \rangle|^2 =$$

$$\frac{W2MOD(K,J,K',J',s)}{XI(J,J')} \; |\langle (J_{core},\ell)K \vdots r \vdots (J_{core},\ell')K' \rangle|^2 =$$

$$\frac{W2MOD(K,J,K',J',s)\; W2MOD(\ell,K,\ell',K',J_{core})}{XI(J,J')\; XI(K,K')} \; |\langle \ell \vdots r \vdots \ell' \rangle|^2$$

for jℓ coupling.

Summing over all z-components of $\vec{J}$ for both initial states and final states and dividing by (2J+1) is equivalent to multiplying by XI(J,J'). (See Condon and Shortley, Equations $7^4 5$ and $9^3 11$)

$$|\ell \; r \; \ell'>|^2 = \frac{1}{4\ell_>^2 - 1} \left[\int_0^\infty R \; R' \; r dr\right]^2$$

(R and R' are radial functions although the quantum numbers pertaining to the radial part have not been written in the above equations.) The final result for $3|<n|z|m>|^2$ summed over final states and averaged over initial states is:

$$\frac{W2MOD(L,J,L',J',S)\; W2MOD(\ell,L,\ell',L',L_{core})}{XI(L,L')} \frac{\left[\int_0^\infty R \; R' \; r dr\right]^2}{(2\ell+1)(2\ell'+1)}$$

for LS coupling, and

$$\frac{W2MOD(L,J,K',J',s)\; W2MOD(\ell,K,\ell',K',J_{core})}{XI(K,K')} \frac{\left[\int_0^\infty R \; R' \; r dr\right]^2}{(2\ell+1)(2\ell'+1)}$$

When these quantities are multiplied by (2J+1) and summed over all possible J and J' in the initial and final multiplets, the result is $\mathcal{G}(\mathcal{M})$ in the notation used by Rohrlich[4] and Griem,[5] the $\mathcal{M}$ standing for "multiplet". $\mathcal{G}(\mathcal{L})\mathcal{G}(\mathcal{M})$ is then (2J+1) times the above quantities, the $\mathcal{L}$ standing for "line". $\mathcal{G}(\mathcal{L})$ obviously was defined to satisfy the rule $\sum_{J\,J'} \mathcal{G}(\mathcal{L}) = 1$.

A sum rule derived from first principles states that $\bar{\nu}|<n|z|m>|^2$ summed over all discrete final states and integrated over continuum final states should equal the Rydberg constant in the same units as $\bar{\nu}$. In the program print out the quantity S3 or SUM3 is the sum over discrete states of $3\,\bar{\nu}|<n|z|m>|^2$ with $\bar{\nu}$ in cm^{-1}. It should approach 329,212.

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[4] F. Rohrlich, Ap. J. 129, 441,449 (1959).

[5] H. Griem, Plasma Spectroscopy, McGraw Hill Book Company, New York (1964).

Intermediate Coupling

Most elements do not fit a well-defined coupling scheme as nicely as might be desired. In other words, their states are mixtures of pure states. No matter what basis is chosen--LS, jl, jj, etc.--the actual states are linear combinations of the basis states, and a transformation matrix between the actual states and the pure states exists.

For the intermediate coupling (IC) program, an LS basis was used, and the elements of the transformation matrix between states of different configurations were assumed to be zero. For each type of configuration involved, a theoretical matrix expression for the electrostatic and spin-orbit perturbations to the Hamiltonian was generated in terms of F_0, G_0, F_2, G_2, ζ, and ζ'. The electrostatic parameters, F_0, G_0, F_2, and G_2, appeared only on the diagonal for the LS basis (See Condon and Shortley, [13]), while the two spin-orbit parameters ζ and ζ' appeared in many off-diagonal positions (Condon and Shortley, [11]). However, no cross terms exist between states of different J, implying that J is a good quantum number in all coupling schemes.

If the theoretical expression is correct and if it is valid to ignore configuration interaction, then it should be possible to choose values for the parameters such that the diagonalized matrix corresponds closely to the observed energies, in spite of the fact that the number of energies in a configuration (the number of conditions that can be imposed on the parameters) is larger than the number of parameters. In practice, the parameters are adjusted to give a least squares fit between the energies calculated by diagonalization and the observed energies. This is done by using trace conditions from the blocks of different J within a configuration (There are no interaction terms between states of different J.) to set several of the parameters initially. As a first guess, the less significant parameters are set equal to zero. The matrix is then diagonalized and partial derivatives of the eigenvalues with respect to the parameters are calculated. A multiple-dimensional Newton's method is applied to readjust the parameters. The process is repeated until the sum of the squares of the energy differences changes by less than 0.1% from its previous value.

The matrix elements for z between various LS states are easy to calculate, although phases are somewhat of a problem. (See Condon and Shortley, [11]). Using the transformation matrices, calculation of oscillator strengths is straightforward.

THE RADIAL INTEGRAL

Schroedinger's equation for the radial wave function is:

$$R = R_{n\ell}/r = P_{n\ell}/r \quad \frac{\partial^2 R}{\partial r^2} + [-2V(r) - \frac{\ell(\ell+1)}{r^2} + \varepsilon]R = 0$$

where r is in Bohr radii

and ε is in Rydbergs

Both of the methods used in these programs for solving this equation, the Bates-Damgaard approximation[6] and the scaled Thomas-Fermi method,[7] are semi-empirical--that is, ε is set equal to the observed energy of a known level. The difference between the two approaches lies in the potential V(r) that is chosen.

The Bates-Damgaard or Coulomb Approximation

As a first approximation one guesses that the potential in which the outer electron moves is simply a Coulomb field due to a nucleus of charge +Z shielded by NEL-1 electrons very close to the nucleus. Thus $V(r) = -\frac{C}{Y}$ where C = Z-NEL+1 is the effective core charge. (C = 1 for neutral atoms.) Letting $\varepsilon = -\frac{C^2}{n^2}$ the differential equation is now:

$$\frac{\partial^2 R}{\partial r^2} + [\frac{2C}{r} - \frac{\ell(\ell+1)}{r^2} - \frac{C^2}{n^2}] R = 0$$

---

[6] D. Bates and A. Damgaard, Phil. Trans. Roy. Soc. (London) 242A, 101 (1949).

[7] J. Stewart and M. Rotenburg, Phys. Rev. 140, A1508 (1965).

There are two boundary conditions, that R→0 at the origin and infinity. They can both be met only when n is an integer. In complex atoms n is generally non-integral, and one condition must be dropped. Since the major contribution to $\int_0^\infty R_n R_m \, rdr$ comes from large r for most transitions, it is reasonable to forget the condition at the origin. The wave function then blows up at zero and is not normalizable.

A mathematical trick is applied at this point. An asymptotic expansion for large r is generated by making the substitution $R=ue^{-\frac{cr}{n}}$ and finding a recursion relation for u.

$$R = e^{-\frac{cr}{n}} \left(\frac{2cr}{n}\right)^n \left[1 + \sum_{t=1} \frac{a_t}{r^t}\right]$$

a_t is given by a recursion relation in reference 6.

As long as the $\sum_t$ contains a finite number of terms, the condition at infinity holds and the one at zero does not. But, a quick check shows that the differential equation has an irregular singularity at infinity. Therefore, a power series expansion in (1/r) does not necessarily converge to a solution. In fact, the sum diverges here. In spite of this, if the series is terminated at the proper term, it gives very good fit to the actual solution for r>2 or 3 (depending upon n and l, of course).

$\int_0^\infty R_n R_m \, rdr$ is now an integral of an exponential term times a power series in r, and may be expressed as a sum of gamma functions. Because the function does not have to be evaluated numerically at a number of points, very rapid computer calculations are possible. (The normalization is also given analytically.[6]) To overcome the problems of the singularity of the origin and of the diverging series, all powers of r less than 2 in the quantity $R_n R_m r$ are removed. These terms do not exist physically since the actual potential is not a Coulomb field near the origin. For the details of the theory and calculation, see References 6 and 8.

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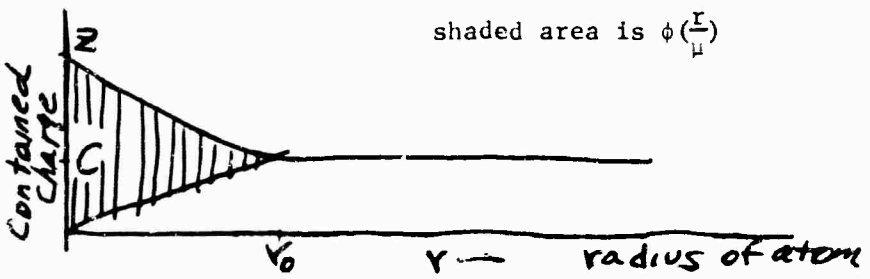
[8] E. Corinaldesi and E. Geil, Computer Program for Bates-Damgaard Integrals, Westinghouse Research Laboratories Scientific Paper 66-1C1-BPLAS-P4 (1966).

The Thomas-Fermi Method

The Thomas-Fermi approach utilizes a somewhat more realistic potential. Instead of assuming that the $N_{el}-1$ shielding electrons are clustered within an infintesimal distance of the nucleus, it predicts a distribution of the shielding electrons based on Fermi-Dirac statistics. The fact that the potentials formed in the above manner bring the wave functions much closer to fitting the boundary condition at the origin justifies the use of the method. Moreover, the fit can be made perfect by linearly expanding or contracting the potential in space by a scaling factor close to one. The latter is the scaled Thomas-Fermi method.

The easiest way to understand the method is to look at the net charge contained within a sphere of radius r as a function of r.



The contained charge must obviously go to Z as $r \to 0$, while for $r > r_o$ -- that is, for r outside of the core--the contained charge is exactly C, as in the Bates-Damgaard method.

$$\text{containing charge} = \begin{cases} Z[\phi(\frac{r}{\mu}) + \frac{Cr}{r_o}] \\ C \end{cases} ; \qquad V(r) = \begin{cases} \dfrac{-Z[\phi(\frac{r}{\mu}) + \frac{Cr}{r_o}]}{r} & r<r_o \\ -C/r & r>r_o \end{cases}$$

where $\phi(0) = 1$, $\phi(x_o) = 0$, $\phi'(x_o) = -\dfrac{C}{x_o Z}$

with $x = \dfrac{r}{\mu}$, $x_o = \dfrac{r_o}{\mu}$

According to Fermi-Dirac theory:

$$\mu = 0.8853 \; Z^{-1/3}$$

$$\frac{d^2\phi}{dx^2} = \phi^{3/2} \; x^{-1/2}$$

At first glance there appears to be one extra boundary condition on the differential equation for ϕ. However, x_o has not been specified, and all three conditions are needed to uniquely determine ϕ. The equation must be solved numerically, but without x_o the calculations are quite extensive. Luckily, the work has already been done, and a polynominal fit for the value of x_o as a function of (C/Z) has been made.[5] The present jl and IC programs merely solve for x_o using the polynomial and then generate ϕ by starting at x_o with $\phi(x_o) = 0$ and $\phi'(x_o) = -\frac{C}{x_o Z} \cdot \phi$ automatically becomes one at zero. This calculation need only be performed once for each atomic species, for ϕ is completely determined by C and Z.

e solution to Schroedinger's equation must also be done numeric No analytical solution is possible because V(r), which depends c ϕ, is on.y known numerically. Two transformations are made:[5]

$$R(r) = p(y^2) \quad , \quad r = y^2 \quad , \qquad R(r) = R(y^2)$$

$$\text{and} \quad p(y) = y^{1/2}\, q(y) \quad , \qquad dr = 2ydy$$

giving:

$$\frac{\partial^2 q}{\partial y^2} = \left\{ \frac{16\,\ell(\ell+1)+3}{4y^2} + 4y^2[2V(y^2) - \varepsilon] \right\} q$$

This is solved by Numerov's method which has an error in each step on the order of h^6 (h = step size). In the program h was $y_o/32$ where $y_o = r_o^{1/2}$.

The integration was started at a y quite a bit larger than y_o by evaluating the asymtotic expansion of the Bates and Damgaard (BD) function at two points separated by h. Care must be taken that y is large enough for the asymtotic expansion to be sufficiently accurate and for the tail of the wave function to be negligible beyond y. Still, the starting point must not be so far out that Numerov's method drifts from the actual solution. The first term of the asymtotic expansion is of the form e^{-y^2}, and such functions do exhibit considerable drift when Numerov's method is started too far out. (The higher derivatives of

e^{-y^2} are very large compared to the function itself when y is large.) In this program the integration was started at the point where the first term of the Bates and Damgaard expansion has dropped to about 1/3000 of its maximum value.

If the scaled Thomas-Fermi method is being done, the integration is stopped at one step from the origin and the number of nodes in the wave function is checked to see if it is equal to $n_{int} - \ell - 1$. n_{int} is the given principal quantum number, not the effective n calculated from $\varepsilon = -\frac{C^2}{n^2}$. n_{int} is always an integer. If the number of nodes is not correct, then the direction in which the scaling factor must be changed is immediately determined. On the other hand, if it is correct, then the ratio of the two points closest to the origin is checked against the ratio predicted by a special asymtotic expansion for small y, obtained from a recursion relation for the approximate equation:

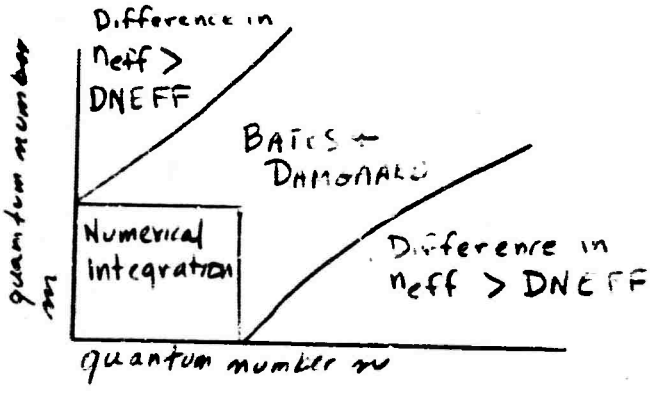
$$\frac{\partial^2 q}{\partial y^2} = \frac{16\,\ell\,(\ell+1)+3}{4y^2} - 8Z\,q$$

From this the direction of the next change is found. The scaling factor steps in the proper direction by 0.05, to either 1.05 or 0.95, and the diff. eqn. is resolved with the appropriately changed potential. The scaling factor continues to move in one direction until the value which gives a boundary fit is overstepped. Then the step size is cut in half each time a new step is made. In this manner, the interval in which the correct value falls is bisected with each step. The iteration goes on until the step size is less than 1/2000 or until the ratio of the two points next to the origin is within one percent of its predicted value.

In the rare gases the ground state has too small an n_{eff} to be put into the Bates and Damgaard (BD) method. Instead the wave function of the ground state is calculated numerically by the scaled Thomas-Fermi method. Therefore, when the ground state is involved the $\int_0^\infty R_n R_m\, r dr$ is done numerically, implying that the wave functions of all upper states that make transitions to the ground state must be known numerically. One way of getting the upper state wave function would be to sum BD

asymtotic expansion at each point desired. However, it is quicker to simply solve Schroedinger's equation numerically since Numerov's method requires only a small number of operations at each point, whereas summing the asymtotic expansion is somewhat involved. As long as the differential equation is being solved numerically, it is just as easy--and certainly more accurate--to use the Thomas-Fermi potential in place of a pure Coulomb potential. This constitutes the unscaled Thomas-Fermi method and has roughly a factor of ten advantage in computer time over the scaled TF method. In general, wave functions generated this way will blow up at the origin and must be chopped off near r = 0. The program imposes the form $r^{\ell+1}$, the first term of the expansion of the wave function for small r, when the centrifugal potential term $\frac{16\ \ell(\ell+1)\ -13}{4y^2}$ begins to dominate.

GIANT/FIASCO first solves for ϕ and then generates a scaled Thomas-Fermi wave function for the ground state and unscaled Thomas-Fermi wave functions for all other states up to the point where n_{eff} is greater than the n_{eff} of the ground state by more than DNEFF an arbitrary limit fed into the program. (Transitions with a difference in n_{eff} greater than DNEFF are not considered. This is true of non-ground state transitions as well.) All generation of any kind of TF wave functions is performed by an internal procedure called THOMASFERMI. The integration of $\int_0^\infty R_n R_m\, r dr$ is carried out numerically when both wave functions are known numerically and is done by the Bates and Damgaard method in other cases. Of course, it is not done at all if the difference in the n_{eff}'s is larger than DNEFF.



There are several arbitrary conditions dealing with the Thomas-Fermi method specifically that are built into the program and may require modification in the futu-e. They are:

1) the step size h for solving differential equations--it is x $x_o/4096$ for ϕ, and $y_o/32$ for the wave functions
2) the conditions ior stopping the itera'ion in the scaled TF method
3) the method of chopping off the singularity at the origin in the unscaled TF process
4) choosing the y outside of y_o at which to start solving Schroedinger's equation
5) deciding which transitions should be done by the BD method and which should be done numerically
6) deciding which levels should be scaled TF and which should be unscaled TF.

SYMBOL TABLE

Program I

Z: the atomic number

NEL: the number of electrons

C: the core charge seen by the outer electron C=Z-NEL+1

R: the Rydberg constant in reciprocal centimeters R=109737.31

N: an index running over the energy levels

L: orbital angular momentum of the outer electron

J: total angular momentum of the atom

T: energy of the level in cm^{-1}

TINF: energy limit of the level in cm^{-1}

In the LS program only

MULT: multiplicity =2S+1 where S is the total spin of the atom

LT: total orbital angular momentum of the atom

P: parity of the state

In the jl and IC programs only

CORE: total angular momentum of the core

K: intermediate quantum number

TINF0: the value of TINF if CORE=1.5 or 0.5

TINF1: the value of TINF if CORE=1.5

TINF2: the value of TINF if CORE=0.5

NEFF: the effective principal quantum number of the outer electron

Program II

L, J, T, MULT, LT, P, CORE, K, and NEFF have the same meaning as in Program I but are now arrays. Z, NEL, and C also have the same meaning.

N: an index running over the states. In particular, it is the index of the initial state when dealing with a transition. In PROCEDURE THOMASFERMI, however, it has the value of NEFF.

M: an index running over the final states.

K: in the LS program only, means the same thing as M does in the jl and IC programs

DNEFF: the largest difference in NEFF for which the program will consider a transition between two levels. Also, in the jl and IC programs, Thomas-Fermi wave functions are calculated for all levels whose NEFF is less than DNEFF&greater than NEFF of the ground state.

NMAX: the highest energy level index to be considered.

NNMAX: the highest energy level index to be considered for the initial state.

OS: the square of the matrix element of $\vec{r}$ summed over the M_j in the final level and averaged over the M_j in the initial level.

LAMBDA: the wavelength in angstroms

TT: the energy of a transition in cm^{-1}

C1: a constant =0.587234

YY: C1 x TT

SUM1: the sum of the OS's for all transitions to a given level

SUM2: the sum of the quantity OS/TT for all transitions to a given level

SUM3: the sum of the quantity OSxTT for all transitions to a given level

S1, S2, and S3 have the same meaning in the LS program.

A: the transition rate in sec^{-1}

I1, I2, and I3 are indices used in the Thomas-Fermi and intermediate coupling sections of the jl and IC programs.

Variables Associated with the Thomas-Fermi Method

QQ: the independent variable in the polynomials used to initialize the ionic radius. See Stewart and Rotenberg,[7] Appendix A.

QQSUM: the sum of the QQ polynomial

XO: the ionic radius times $Z^{1/3}$ /0.8853

AA, BB, and CC: the coefficients in the initialization polynomials

PHIM1, PHIO, and PHIP1 are ϕ_{i+1}, ϕ_i, and ϕ_{i-1} respectively. The ϕ-function is found by solving the differential equation $\phi''(x) = [\phi(x)/x]^{1/2}$ from x_o inward.

H: the step size used in this iteration. It is = to XO/4096.

H32: a variable = to $H^{3/2}$

HSTAN: the step size used in solving for the actual wave functions. It is = to $\sqrt{r_o}/32$. The independent variable in the wave function is $y=\sqrt{r}$

VMOD: $8y^2$ times the Thomas-Fermi potential in Rydbergs. It is given as a function of y, at points separated by HSTAN/2.

WF: a 2-dimensional array giving $R(y^2)/\sqrt{y}$ as a function of the index of the energy level and y, at points separated by HSTAN.

NORM: the normalization factor by which WF for a given level must be multiplied.

NTF: the index of the highest energy level for which a Thomas-Fermi wave function is calculated

NPOINTS: for each level, the number of points at which WF is given. It is = to the maximum y considered divided by HSTAN.

NINT: the principal quantum number of the outer electron for a given state. (NINT stands for N integral, as opposed to N effective.) The number of nodes expected in the wave function is NINT-L-1.

The following variables are declared inside PROCEDURE THOMASFERMI.

WFP1, WF0, and WFM1: values of WF around a given y

KSP1, KS0, and KSM1: values of K_s where the differential equation is

$$\frac{d^2}{dy^2} WF(y) = K_s(y).$$

FACTORP1, FACTOR0, and FACTORM1: values of the quantity $(1 - H^2K_s/12)$

Note: P1 and M1 stand for +1 and -1. P1 means that the value is given for a y one step closer to the origin, while M1 corresponds to a y one step farther from the origin. (The integration proceeds inward.)

EPSILON: the energy eigenvalue in Rydbergs.

H (already declared outside the procedure): the step size used in solving for WF. It is readjusted as the scale factor a is varied.

H2: a variable set equal to H^2

H2T4: $4H^2$

H2012: $H^2/12$

H2T506: $5H^2/6$

Y2T4: $4y^2$

RMAX: the largest value of r considered. Outside of RMAX the wave function is assumed to be too small to make any significant contribution.

INVR: 1/RMAX

SCALE: the scale factor a in the scaled Thomas-Fermi method

JUMP: the amount by which SCALE is varied between successive trials.

DIRECTION: the direction in which SCALE is varied. It is +1 for an increase and -1 for a decrease.

OLDDIRECTION: the previous value of DIRECTION

BEFORE: a Boolean variable which is true as long as SCALE continues to jump in one direction by steps of 0.05. When the proper value of SCALE has been overstepped, BEFORE becomes false, SCALE converges by a bisection procedure.

LASTTIME: a Boolean variable which becomes true when SCALE has converged sufficiently. It activates the normalization and cut-off procedures.

VARYSCALE: a Boolean variable which determines whether a scaled or unscaled Thomas-Fermi method is to be used. In the present program VARYSCALE is true only for the ground state.

NEW12: the number of points at which WF is known after it has been interpolated so that the spacing between points is HSTAN

LPOLY: a function of L which is used a large number of times. It is = to 16L(L+1)+3.

NODES: the number of times that the wave function crosses the axis each time the differential equation is solved.

RATIO: the ratio of the values of the wave function between the two points closest to the origin.

DRATIO: the change in RATIO between two successive iterations.

INSIDE: a variable which--on the last iteration--goes to true as soon as y moves from the exponential region into the oscillatory region.

NORMOD: a non-array quantity which is summed to form the array NORM, the normalization factor.

Variables Associated with Intermediate Coupling

(Not all of the variables declared are described here, but most of the important ones are mentioned.)

SPORBMATRIX (4D or 3D): the coefficients of the first spin-orbit parameter in the theoretical Hamiltonian matrix. In the 4D case, the first index is the ℓ of the configuration, the second index is the J, and the last two are the row and the column within a J-block. The 3D (i.e. 3-dimensional) array is missing the first index.

SPORBMATRIXP (4D or 3D): the coefficients of the second spin-orbit parameter in the Hamiltonian.

ELECMATRIX (4D or 3D): the theoretical Hamiltonian for the electrostatic parameters. In the 4D array, the first three indices are the same as in SPORBMATRIX4D while the last index identifies the electrostatic parameter under consideration. No column index is necessary since the electrostatic interaction is diagonal in the LS basis.

IELEC and NELEC: the index and total number of the electrostatic parameters.

IPARAM and NPARAM: the index and total number of parameters.

ELECPARAM: an array containing the values of the electrostatic parameters as they are adjusted by PROCEDURE DIAG.

SPORBPARAM and SPORBPARAMP: the values of the two spin-orbit parameters.

IGREATER: the greater of the two ℓ's of two states under consideration.

STLS3D: the matrix elements of cosθ between pairs of LS states. The first index is LGREATER and the other two are the rows and columns.

J2, J3, S2, S3, L2, and L3: the variables used to represent quantum numbers in generating the Hamiltonian matrices and the LS strengths.

HOLD: the variable that holds on to the value of L as the energy levels are read in. When the end of a configuration is reached, the next L is no longer = to HOLD and PROCEDURE DIAG is called.

T2D and N2D: arrays holding the values of T and N for the levels of a given configuration. The first index is the J of the level and the second puts the states of a given J-block in order of increasing energy.

IJ, IJMIN, and IJMAX: the index and limits for the J-blocks of a given configuration.

INDEX and BLOCK: arrays over N giving the J-block and the position in that block of every level fed into the program. The number BLOCK is distinct from one configuration to the next.

LOWERBLOCK: the lowest BLOCK in a given configuration.

SIZE2 and SIZE3: the sizes of the J-blocks as predicted by the sections which generate the theoretical Hamiltonian matrices and the LS strengths.

SIZE: the size of the J-blocks in the observed levels which are read by the program.

I2LOWER and I3LOWER: integer arrays which indicate what position in the STLS3D matrix to look for a given pair of L's and J's.

TRACE and TRACES: the traces of the J-blocks. Since the traces of the undiagonalized theoretical Hamiltonian and the traces of the observed energy matrix should be the same, enough information is present to initialize the values of the parameters for a given configuration.

H: a matrix for the Hamiltonian formed from the theoretical expressions for the Hamiltonian and the values which the parameters happen to have at the moment.

TCALC: an array containing the energies calculated by diagonalizing the H-matrix.

V3D, V2D, and VTEMP: various forms of the matrix which diagonalizes the Hamiltonian.

DERIV: a matrix of the derivatives of the calculated energy eigenvalues with respect to the parameters.

ALPHS: the coefficients of the set of simultaneous equations which are solved for the corrections to the parameters. They are calculated from the DERIV's and the differences between the observed and calculated T's.

IT: the number of times that the parameters for a configuration have been readjusted for a better least-squares fit to the observed energies.

SUMSQUARES: the sum of the squares of the differences of the observed and calculated energies.

HOLDSUM: the value of SUMSQUARES from the previous iteration. If SUMSQUARES has changed by less than 0.1%, the iteration is terminated.

REAL PROCEDURE XI is the same as -(J, J')

$$= \begin{cases} (J+1)(2J+3) & \text{if } J' = J+1 \\ J(J+1) & J' = J \\ J(2J-1) & J' = J-1 \end{cases}$$

REAL PROCEDURE W2MOD is a modified Racah coefficient squared.

$$W2MOD(L, J, L', J', S) = (2J'+1)\,L\,(2L+1)(2L'+1)\,W^2(L, J, L', J'; S)$$

Moreover,

$$\frac{W2MOD(1, J, L', J', S)}{XI(J, J')} = \frac{|\langle SLJ\ P\ SL'J'\rangle|^2}{|\langle L\ P\ L'\rangle|^2}$$

where $\vec{P}$ is class $\vec{T}$ with respect to $\vec{J}$ and $[\vec{S}, \vec{P}] = 0$

REAL PROCEDURE I calculates the radial integral $\int R_n(r)R_m(r)\,rdr$ by numerical integration if both N and M are less than the index of the highest state for which a Thomas-Fermi wave function has been calculated. For all other pairs the Bates-Damgaard method of integration is called through REAL PROCEDURE BD.

PROCEDURE THOMASFERMI takes NEFF, NINT, and L for the Kth level and produces a wave function.

PHI/GENERATOR produces the Thomas-Fermi potential by numerically solving a differential equation derived from the theory. All quantities calculated in this section pertain to all levels for which PROCEDURE THOMASFERMI is applied.

Section in the program which sets NINT[N] for all the energy levels for which Thomas-Fermi wave functions are calculated must be changed for every different atomic or ionic species.

The IC Program

MATRIX/GENERATOR - the part of program which generates the theoretical expressions for electrostatic and spin-orbit perturbations to the Hamiltonian. The LS basis is used and matrices similar to those on pages 268-269 of Condon and Shortley [11] are produced for each parameter. Section 1[13] page 299 gives the actual coefficients generated, since the program is at present designed to do the rare gases.

LS/STRENGTHS - produces a matrix for the angular part of the dipole operator. All possible pairs of LS states are considered. When PROCEDURE DIAG has expressed each energy level as a linear combination of LS states, it is then easy to calculate the angular matrix element between any two of the actual states.

A section in the program takes the energy levels in each configuration as a group, places them in blocks of different J, and then re-orders each J-block in order of increasing energy, which are then fed into PROCEDURE DIAG, one configuration at a time.

PROCEDURE DIAG takes each configuration fed into it and compares the actual observed energies with the theoretical expressions for the Hamiltonian which have been generated by MATRIX/GENERATOR. DIAG then adjusts the theoretical parameters so that the diagonalization of the theoretical Hamiltonian gives a least-squares fit to the observed energy eigenvalues. Once this is done, the matrix which diagonalizes the Hamiltonian is merely an expansion of the observed levels in terms of LS basis states. This matrix saved for the final computation of the oscillator strengths.

INPUTS TO PROGRAMS 1 AND 2 OF GIANT/FIASCO (LS PROGRAM)

under "FIASCO" (input to Program 1):

a card with Z, the atomic number and N_{el}, the number of electrons

a card with the value of T_{inf}

for each level of Moore's tables a card giving:

L (orbital angular momentum of the outer electron)

MULT (multiplicity = 2S + 1)

LT (total orbital angular momentum)

P (parity + +1 even, = -1 odd)

J (total angular momentum)

T (energy of the level in cm^{-1})

under "READER2" (input to Program 2):

a card with NMAX (the maximum N to be read) and NNMAX (max on the index of the initial state)

a card with DNEFF (the limitation on interacting levels)

INPUTS TO PROGRAMS 1 AND 2 OF GIANT/FIASCO (jl and IC PROGRAM)

under "FIASCO" (input to Program 1):

a card with Z, the atomic number and N_{el}, the number of electrons

a card with the value of T_{inf} for CORE = 0, the value of T_{inf} for CORE = 1.5, the value of T_{inf} for CORE = 0.5

for each level of Moore's tables a card giving:

CORE (total angular momentum of the core)

L (orbital angular momentum of the outer electron)

K (intermediate quantum number)

J (total angular momentum)

T (energy of the level in cm^{-1})

under "READER2" (input to Program 2):

a card with NMAX (the maximum N to be read)

a card with DNEFF (the limitation on interacting levels)

15 cards giving the coefficients of the three initialization polynomials for the Thomas-Fermi function. Each card has four numbers:

the index of the coefficient,

A(index),

B(index),

C(index),

(See Stewart and Rotenberg[5], Appendix A)

and, <u>for the IC program only</u>, for each possible L (L = 0, 1, 2, 3) a card with:

LM1 (coeff of F_2 if $L_{total} = L - 1$),

LSAME (coeff of F_2 if $L_{total} = L$),

LP1 (coeff of F_2 if $L_{total} = L + 1$),

LM1SC (coeff of G_0 if $L_{total} = L - 1$ and S = 0),

LP1SO (coeff of G_2 if $L_{total} = L + 1$ and S = 0),

(See Condon and Shortley, pp 2[illegible]-299).

ON EXTENDING PROGRAMS 1 AND 2

LS Program: For elements in which the L of the parent term is non-zero, the expression for OS must be changed from W2MOD (1, J, L', J', S)σ^2 to

$$W2MOD(L, J, L', J', S)\,\frac{W2MOD(1, L, 1', L', L_{parent})}{XI(L, L')}\,\sigma^2$$

In more complex elements, coefficients of fractional parentage must also be added.

jl and IC Programs: To do other rare gases, the only change necessary is the setting of NINT (the principal quantum number) for all of the levels to be done by Thomas-Fermi method.

To do other elements the cards which define the ground state as a $^1S_0$ state and multiply the strengths of ground state transitions by six, must be altered.

IC Program: NMAX must be set low enough that no configuration with fewer than the predicted number of levels gets read by Program 2. NMAX should be one greater than the last level in the highest configuration to be done. Although this greatly limits the IC Program, it would be possible to do many more transitions if PROCEDURE DIAG expanded the actual states in terms of jl basis states instead of LS states. Higher states in incomplete configurations could then be approximated as pure jl states. Therefore, a matrix which transforms the LS basis to the jl basis would be a useful addition.

For elements with more complex configurations, the variables which identify the states and the J-blocks must be changed, along with the generator of the theoretical Hamiltonian and the LS strengths. This involves rewriting most of the procedures.

OUTPUT FROM PROGRAM 2 OF GIANT/FIASCO

Following the listing of the energy levels from Program 1, Program 2 will print out varying quantities of fairly self-explanatory information, depending upon the coupling scheme--that is, LS, jl, or IC.

The jl and IC programs will first list all the Thomas-Fermi wave functions as a function of the number of steps from the origin in y. (The function printed is actually q(y); see the section describing GIANT/FIASCO.) Note that the first ten steps are given, and then jumps of five steps are taken to save space. Immediately below each wave function is printed the expected number of nodes, which is simply $n_{int}-l-1$, and the actual number of nodes in the wave function shown. The two numbers are always the same for levels done by the scaled TF method, but in the unscaled cases (These can be identified by the fact that SCALE = 1.000.) there is no guarantee that this is so. When the two are the same, it is an indication that the Thomas-Fermi method is valid.

The IC program will now print out the transformation matrices from LS states to the observed states. Double lines separate different configurations, while single lines separate the iterations approaching a leastsquares fit for a given configuration. For each block of a different J, the observed energies and the energies calculated by diagonalizing the theoretical Hamiltonian appear next to the corresponding rows of the transformation matrix. (Note that some of the matrices are rectangular although all of them should be square. Extra columns on the <u>right</u> should be ignored.) Directly below, and within the same J block, are the derivatives of the calculated energy eigenvalues with respect to the various adjustable parameters. The rows are in order of increasing energy eigenvalues, and the columns are in the same order as the list of parameters, which appears once for each iteration. (Derivatives for parameters which are not involved--that is, parameters which are zero after the first iteration--should be ignored.)

Finally, the LS, jl, and IC programs all print out the transition probabilities in the form $3|\langle n|z|m\rangle|^2$, which had already been summed

over final states for m and averaged over initial states for n. At the far right is Einstein's spontaneous emission coefficient in the form $A_{nm} \times 10^{-8}$. However, at present the jl and IC programs have a card near the end of Program 2 which reads:

```
A←Ax(2xJ(N)+1/(2xJ(M)+1);
```

This reverses the indixes n and m so that $A_{mn} \times 10^{-8}$ is printed out instead of $A_{nm} \times 10^{-8}$ as the comment cards in Program 2 claim.

AUXILIARY PROGRAM FIASCO/RESULTS

This program merely reads the stored output of Program 2 from the disc READF2 and prints out the transition probabilities in several forms. GF is gf, FNM is f_{nm}, ANM is A_{nm}, and AMN is A_{mn}. Input is just the levels of Moore's tables with the same cards that go into Program 1.

```
13113A1A5 WEDNESDAY, MAY 10, 1967                   NRL ALGOL VERSION OF  5/01/67
      BEGIN

   FILE OUT PRINTER R(2,15);                                               SC   11    010
   FILE OUT READF1 DISK SERIAL[20:60] "ICAE" "READF1"(2,10,300,SAVE 30) ;  START OF SEGMENT **********    2
   FILE OUT READF2 DISK SERIAL[20:60] "ICAE" "READF2"(2,10,300,SAVE 30) ;  SC   21    010
   BEGIN                                                                   2C   21    312
   COMMENT IMPACT BROADENING AND SHIFT OF SPECTRAL LINES BY ELECTRONS     2C   21    710
           ---PROGRAM I---FOR HEAVY ELEMENTS (TENTATIVE)---                SC   21   1012
           INPUT: CARD WITH Z (ATOMIC NUMBER) AND NEL (NUMBER OF ELECTRONS) SC  21   1012
                  ACARD WITH TINF FOR CORE=0, TINF FOR CORE=1.5,           SC   21   1012
                     TINF FOR CORE=0.5,                                    SC   21   1012
                  A CARD FOR EACH LEVEL OF MOORES TABLES GIVING:           SC   21   1012
                  CORE (TOTAL ANGULAR MOMENTUM OF THE CORE),               SC   21   1012
                  L (ORBITAL ANGULAR MOMENTUM OF OUTER ELECTRON),          SC   21   1012
                  K (INTERMEDIATE QUANTUM NUMBER),                         SC   21   1012
                  J (TOTAL ANGULAR MOMENTUM),                              SC   21   1012
                  T (ENERGY OF LEVEL)                                      2C   21   1012
          OUTPUT:TABLE GIVING Z, NEL AND C=Z-NEL+1                         SC   21   1012
                  AND, FOR EACH LEVEL,                                     SC   21   1012
                  N (INTEGER NUMBERING LEVEL, FOR REFERENCE),              SC   21   1012
                  NEFF (EFFECTIVE PRINCIPAL QUANTUM NUMBER                 SC   21   1012
                       OF OUTER ELECTRON),                                 SC   21   1012
                  CORE,L,K,J,T,TINF,                                       SC   21   1012
                  CARD WITH Z,NEL,C                                        SC   21   1012
                  A CARD FOR EACH LEVEL GIVING:                            SC   21   1012
                  N,NEFF,CORE,L,K,J,T;                                     2C   21   1012
  FILE IN READER "FIA2CO" (2,10);                                          SC   21   1012
                                                                           SC   21   1012
  FORMAT F1("Z=",I2,X4,"NEL=",I2,X4,"C=Z-NEL+1=",I2),                      SC   21   1012
                                                              START OF SEGMENT **********    3
        F2(X2,"N",X8,"NEFF",X7,"CORE",X4,"L",X4,"K",X4,"J",X8,"T",X13,     SC   31    312
           "TINF"),                                           START OF SEGMENT **********    4
        F3(I3,X4,R14.11,X4,R3.1,X3,I2,X2,R3.1,X2,R3.1,X3,R12.3,X3,R12.3),  SC   A1    312
        FR(I2,",",I2,",",I2,",",),                                         SC   A1    312
       F5(I3,",",R14.11,",",R3.1,",",I2,",",R3.1,",",R3.1,",",R12.3,",",); SC   A1    312
  LABEL START,EXIT;                                                        2C   A1    312
                                                                           SC   A1    312
  INTEGER Z,NEL,L,C,N;                                                     SC   A1    312
  REAL TINF0,TINF1,TINF2;                                   A 13   75 LONG, NEXT SEG    3
  REAL CORE,K,J,T,TINF,NEFF,R;                                             SC   31    312
  R=109737.21;                                                             SC   31    312
  READ (READER,/,Z,NEL);                                                   SC   31    312
  C=Z-NEL+1;                                                               SC   31    312
  WRITE (PRINTER[DBL],F1,Z,NEL,C);                                         SC   31    811
                                                                           2C   31   1513
                                                                           SC   31   1712



  WRITE (READF1,FR,Z,NEL,C);
  WRITE (PRINTER[DBL],F2);                                                 2C   31   3011
  N=0;                                                                     SC   31   A311
  READ(READER,/,TINF0,TINF1,TINF2);                                        SC   31   A411
  START:  READ(READER,/,CORE,L,K,J,T)[EXIT];                               SC   31   A710
  IF CORE=1.5 THEN TINF=TINF1 ELSE                                         SC   31   9013
  IF CORE=0.5 THEN TINF=TINF2 ELSE                                         SC   31   7513
  TINF=TINF0;                                                              SC   31   7713
  NEFF=C×SQRT(R/(TINF-T));                                                 SC   31   8210
  N=N+1;                                                                   SC   31   8A13
  WRITE (PRINTER,F3,N,NEFF,CORE,L,K,J,T,TINF);                             SC   31   8712
  WRITE (READF1,F5,N,NEFF,CORE,L,K,J,T);                                   SC   31   8813
  GO TO START;                                                             SC   31  10711
  EXIT:          REWIND (READF1);              END;                        SC   31  12511
                                                                           SC   31  12813
  BEGIN                                                    3 13  131 LONG, NEXT SEG    2
  FILE IN READER "READER2" (2,10);                                         SC   21   1110
                                                                           SC   21   1110
  COMMENT IMPACT BROADENING AND SHIFT OF SPECTRAL LINES BY ELECTRONS  START OF SEGMENT **********    5
          ---PROGRAM II---FOR HEAVY ELEMENTS (TENTATIVE)---                SC   51    312
          INPUT: CARD WITH NMAX (= MAXIMUM N TO BE READ)  AND NNMAX        SC   51    312
              (= MAXIMUM N TO BE CONSIDERED FOR THE INITIAL STATE),        SC   51    312
                CARD WITH ONEFF (LIMITATION ON INTERACTING LEVELS)         SC   51    312
                AND, 1A CARDS GIVING THE COEFFICIENTS OF THE 3             SC   51    312
                INITIALIZATION POLYNOMIALS OF THE THOMAS-FERMI FUNCTION.   SC   51    312
                EACH CARD HAS 4 NUMBERS:                                   SC   51    312
                   THE INDEX OF THE COEFF, A(INDEX), B(INDEX), C(INDEX),   SC   51    312
                AND, FOR EACH POSSIBLE L (L=0,1,2,3) A CARD WITH:          SC   51    312
                   LM1,LSAME,LP1,LM1SO,LP1SO,                              SC   51    312
                THESE ARE THE COEFFICIENTS IN THE  ELECTROSTATIC MATRIX.   SC   51    312
                (LM1=COEFF OF F2 IF LT=L-1,                                SC   51    312
                 LP1=COEFF OF F2 IF LT=L+1,                                SC   51    312
                 LSAME=COEFF OF F2 IF LT=L,                                SC   51    312
                 LM1SO=COEFF OF G0 IF LT=L-1 AND S=0,                      SC   51    312
                 LP1SO=COEFF OF G2 IF LT=L+1 AND S=0),                     SC   51    312
                FROM PROGRAM I:                                            SC   51    312
                CARD WITH Z,NEL,C                                          SC   51    312
                A CARD FOR EACH LEVEL WITH N,NEFF,CORE,L,K,J,T.            SC   51    312
                (CARDS WITH N>NMAX WILL NOT BE READ)                       SC   51    312
        OUTPUT: TABLES GIVING Z,NEL,C,NMAX,ONEFF,                          SC   51    312
                AND, FOR EACH NUMERICALLY GENERATED WAVE FUNCTION          SC   51    312
                A TABLE OF R(Y*2)/SQRT(Y) VERSUS THE NUMBER OF STEPS OF    SC   51    312
                SIZE H THAT Y HAS TAKEN FROM Y=0                           SC   51    312
                WHERE R IS THE RADIAL WAVE FUNCTION AND Y=SQRT(RADIUS),    SC   51    312
                AND, FOR THE GENERATION OF THE JC COUPLING MATRICES:       SC   51    312
```

```
                  A DOUBLE LINE EACH TIME A NEW CONFIGURATION BEGINS              SC   5:   312
                  A SINGLE LINE EACH TIME THE DIAGONALIZATION OF A                SC   5:   312
                     CONFIGURATION IS REITERATED TO GIVE A BETTER                 SC   5:   312
                     LEAST-SQUARES FIT                                            SC   5:   312
                  FOR EACH BLOCK OF A DIFFERENT J WITHIN A                        SC   5:   312
                  CONFIGURATION, A TABLE GIVING:                                  SC   5:   312
                     FOR EACH ENERGY LEVEL INVOLVED:                              SC   5:   312
                        TOBSERVED, TCALCULATED BY DIAGONALIZATION, AND            SC   5:   312
                        THE CORRESPONDING ROW OF THE TRANSFORMATION               SC   5:   312
                        MATRIX V                                                  SC   5:   312
                     AND BELOW THIS, A MATRIX OF THE DERIVATIVES OF THE           SC   5:   312
                     EIGENVALUES WITH RESPECT TO THE VARIOUS PARAMETERS           SC   5:   312
               AND, FOR EACH LEVEL:                                               SC   5:   312
               N,M,OS,YY,LAMBDA,A*R*R   FOR ALL STATES M INTERACTING              SC   5:   312
                                 WITH N UNDER LIMITATION ONEFF                    SC   5:   312
               AND         N,SUM1,SUM2,SUM3                                       SC   5:   312
               (SUM1=SUM OS(M), SUM2=SUM (OS(M)/(T(M)-T(N))),                     SC   5:   312
               SUM3=SUM (OS(M)*(T(M)-T(N))), A IS THE EINSTEIN A FOR              SC   5:   312
               TRANSITIONS FROM N TO M,                                           SC   5:   312
               OS  = Y*(N1Z1M)*2    )                                             SC   5:   312
               CARD WITH Z,NEL,C,NMAX,ONEFF,                                      SC   5:   312
               AND, FOR EACH LEVEL N,                                             SC   5:   312
                A CARD WITH     N,0,CORE,L,K,J,T,                                 SC   5:   312
               A CARD WITH     N,N,SUM1,SUM2,0,0,0,                               SC   5:   312
               A CARD FOR EACH LEVEL M INTERACTING WITH N (M=N AND M=0)           SC   5:   312
               WITH            N,M,OS(M),YY(M),0,0,0,      )                      SC   5:   312
FORMAT F1(X2,"Z=",I2,X4,"NEL=",I2,X4,"C=",I2,X4,"NMAX=",I3,X4,"ONEFF=",           SC   5:   312
                                                                 START OF SEGMENT **********    6
        I2),                                                                      SC   6:   312
FL("********************************* **********************************"),      SC   6:   312
FPARAM("PARAMETERS     ",A R11,4),                                                SC   6:   312
FIJ("BLOC=",I4),                                                                  SC   6:   312
FV(2R15,3,X10,R20,11),                                                            SC   6:   312
FDERIV(R20,11),                                                                   SC   6:   312
FCHECK(X10,"HD=",R20,11,X5,"YM=",R20,11,X5,"CT=",I3),                             SC   6:   312
FERROR("DET OF AN SMEQ STATEMENT IS ZERO"),                                       SC   6:   312
FSUM("SUMSQUARES=",R20,11,X10,"ITERATIONS=",I2),                                  SC   6:   312
FTF("N=",I3,X4,"NEFF=",R14,11,X6,"SCALE=",R13,11,X4,"STEP SIZE R=",               SC   6:   312
      R13,11),                                                                    SC   6:   312
FRF(X10,I3,E20,10),                                                               SC   6:   312
FNNN("NORM=",R15,11,X6,"EXPECTED NO. OF NODES=",I2,X4,                            SC   6:   312
      "ACTUAL NO. OF NODES=",I2),                                                 SC   6:   312
      F2(I2,",",I2,",",I2,",",I3,",",I2,","),                                     SC   6:   312
      F3("N=",I3,X3,"SUM1=",R20,11,X4,"SUM2=",R20,11,X4,"SUM3=",                  SC   6:   312
         R20,11),                                                                 SC   6:   312


      F4(X4,"N",X7,"M",X10,"3( IZI )*2",X18,"YY",X14,"LAMBDA",X15,                SC   6:   312
           "A*R*R"),                                                              SC   6:   312
      F5(X2,I3,X5,I3,X7,R20,11,R20,11,R20,11,R20,11),                             SC   6:   312
      F6(I3,",",I3,",",R20,11,",",R20,11,",0,0,0,"),                              SC   6:   312
      F7(I3,",",",",R3,1,",",I2,",",R3,1,",",R3,1,",",R12,3,",")                  SC   6:   312
                                                           6 IS  205 LONG, NEXT SEG     5
REAL DD,DGSUM,X0,PHI0,PHI01,RHI01,H,H32,HSTAN;                                    SC   5:   312
ARRAY AA,BB,CC[0:15],RF[0:400,0:250],VMOD[0:500],NORM[0:100];                     SC   5:   312
INTEGER I1,I2,I3;                                                                 SC   5:   1111
INTEGER NTF;                                                                      SC   5:   1111
INTEGER ARRAY NPOINTS[0:100];                                                     SC   5:   1111
INTEGER ARRAY NINT[0:400];                                                        SC   5:   1310
REAL SP,SPP,G;                                                                    SC   5:   1413
ARRAY SPORBMATRIXAD,SPORBMATRIXRAD[0:3,0:5,0:4,0:4];                              SC   5:   1413
INTEGER HOLD,IELEC,J2,L2,L3,J2,S3;                                                SC   5:   1712
INTEGER LR1,LSAME,LR1,LR150,LP150;                                                SC   5:   1712
INTEGER ARRAY ELECMATRIXAD[0:3,0:5,0:4,0:8],I2MAX[0:3,0:5];                       SC   5:   1712
ARRAY T20,N20[0:10,0:5];                                                          SC   5:   2210
INTEGER LOWERBLOCK,IJMAX,IJMIN,IJ;                                                SC   5:   2411
INTEGER ARRAY IMAX[0:10],INDEXBLOCK[0:400];                                       SC   5:   2411
REAL STL3;                                                                        SC   5:   2810
ARRAY STLS3D[0:3,0:12,0:12];                                                      SC   5:   2810
INTEGER J3,LGREATER;                                                              SC   5:   3011
INTEGER ARRAY I2LOWER,I3LOWER[0:3,0:5];                                           SC   5:   3011
ARRAY V10[0:5],V30[0:200,0:5,0:5];                                                SC   5:   3212
INTEGER SIZE2,SIZE3,I2LOWER00,I3LOWER00;                                          SC   5:   3412
REAL SUM1,SUM2,SUM3,C1,C3,TT,YY,LAMBDA;                                           SC   5:   3612
REAL A;                                                                           SC   5:   3612
ARRAY NEFF,CORE,K,J,T[0:400];                                                     SC   5:   3612
INTEGER NMAX,NNMAX,ONEFF,Z,NEL,C,N,M;                                             SC   5:   3911
INTEGER ARRAY L[0:400];                                                           SC   5:   3911
COMMENT DARTIME;                                                                  SL   5:   4110
                                                               ********  SC   5:   4110
COMMENT GAMMA;                                                 00000000  SL   5:   4110
                                                               ********  SC   5:   4110
COMMENT NEWSMFU;                                               00000000  SL   5:   4110
                                                               ********  SC   5:   4110
COMMENT JACOBI;                                                00000000  SL   5:   4110
                                                               ********  SC   5:   4110
REAL PROCEDURE MAX(P,Q); VALUE P,Q; REAL P,Q;                                     SC   5:   4110
BEGIN IF P>Q THEN MAX=P ELSE MAX=Q END;                                           SC   5:   4110
REAL PROCEDURE  XI(J,JP);  VALUE J,JP;  REAL J,JP;                                SC   5:   4710
BEGIN IF JP=J+1 THEN XI=(J+1)*(2*J+3) ELSE                                        SC   5:   4710
      IF JP=J THEN XI=J*(J+1) ELSE                                                SC   5:   4112
      XI=J*(2*J-1);  END;                                                         SC   5:   4510
```

```
REAL PROCEDURE W2WOD(L,J,LP,JP,S); VALUE L,LP,J,JP,S;
REAL L,LP,J,JP,S;                                                                    SC   5:  6010
BEGIN REAL NUM,D;                                                                    SC   5:  6010
                                                                                     SC   5:  6010
      IF JP=J+1 THEN D+JP*(2*J+1) ELSE                       START OF SEGMENT **********    11
      IF JP=J THEN D+J*(J+1) ELSE                                                    SC  11:   010
      D+J*(2*J+1);                                                                   SC  11:   410
IF LP=L+1 THEN                                                                       SC  11:   712
      IF JP=J+1 THEN NUM+(JP+S+LP)*(JP+S+LP+1)*(JP+S+L)*(JP+S+LP) ELSE               SC  11:  1011
      IF JP=J THEN NUM+(J+S+LP)*(J+S+LP+1)*(S+LP-J)*(J+S+L) ELSE                     SC  11:  1112
      NUM+(S+L+JP)*(J+S+L)+(S+LP+JP)*(JP+S+L)                                        SC  11:  2012
ELSE IF LP=L THEN                                                                    SC  11:  2010
      IF JP=J+1 THEN NUM+(JP+S+L)*(JP+S+L+1)*(S+L+J1*1JP+S+L1 ELSE                   SC  11:  3412
      IF JP=J THEN NUM+(J*(J+1)+S*(S+1)+L*(L+1))+2 ELSE                              SC  11:  3710
      NUM+(J+S+L)*(J+S+L+1)*(S+L+JP)*(J+S+L)                                         SC  11:  4410
ELSE                                                                                 SC  11:  5310
      IF JP=J+1 THEN NUM+(S+L+J1*(JP+S+L)*(S+L+JP1*(JP+S+LP1 ELSE                    SC  11:  5010
      IF JP=J THEN NUM+(J+S+L)*(J+S+L+1)*(S+L+J)*1J+S+LP1 ELSE                       SC  11:  A011
      NUM+(J+S+L1*(J+S+L+1)*(JP+S+L)*1J+S+L));                                       SC  11:  6813
W2WOD+NUM/(A*D)); END;                                                               SC  11:  7711
                                                                                     SC  11:  8A12
REAL PROCEDURE LAG ( X , X0 , DX , Y , N ) ;                       11 IS   59 LONG, NEXT SEG     5
COMMENT ORDER 3 LAGRANGE INTERPOLATION, EQUAL INDEPENDENT STEP,       LAG  1  SC   5:  5010
SINGLE DEPENDENT,INDEPENDENT VARIABLE,EXTRAPOLATE IF NOT X0$X$X0+N*DX,  LAG  2  SC   5:  6010
X  = DESIRED INDEPENDENT VALUE                                        LAG  3  SC   5:  A010
X0 = FIRST INDEPENDENT VALUE OF Y TABLE (FOR Y[0])                    LAG  4  SC   5:  A010
DX = TABLE STEP FOR INDEPENDENT                                       LAG  5  SC   5:  A010
Y  = NAME,DEPENDENT VARIABLE VALUE TABLE (MUST BE SINGLE SUBSCRIPT)   LAG  6  SC   5:  6010
N  = MAX INDEX OF Y TABLE ( 2 4 ) ;                                   LAG  7  SC   5:  6010
    VALUE X , X0 , DX , N ;                                           LAG  8  SC   5:  6010
    REAL X , X0 , DX ; INTEGER N ; ARRAY  Y[0] ;                      LAG  9  SC   5:  A010
    BEGIN                                                             LAG 10  SC   5:  4010
        INTEGER I ; REAL S ;                                          LAG 11  SC   5:  6010
                                                                      LAG 12  SC   5:  6010
        IF (I + ENTIER((X - X0)/DX - 1)) < 0 THEN I + 0 ELSE   START OF SEGMENT **********    12
            IF I + 3 > N THEN I + N - 3 ;                             LAG 13  SC  12:   010
        S + (X - X0)/DX - ) ;                                         LAG 14  SC  12:   510
        LAG + ((Y[I + 3] * S - Y[I]) * (S - 3)) * ((S - 3) * S + 2)/3  LAG 15  SC  12:  1010
            + (Y[I + 1] + (S - 2] - Y[I + 2] * (S - 1]) * (S - 3)) * S)/2  LAG 16  SC  12:  1211
    END LAG ;                                                         LAG 17  SC  12:  1712
                                                                      LAG 18  SC  12:  2410
REAL PROCEDURE BO(N,L,N1,L1,C);                                    12 IS   28 LONG, NEXT SEG     5
VALUE N,L,N1,L1,C;REAL N,N1;INTEGER L,L1,C;BEGIN                                     SC   5:  6010
INTEGER T,T1;                                                                        SC   5:  4010
                                                                                     SC   5:  6010
                                                             START OF SEGMENT **********    13


REAL NCN,M,X,Y,Z,SUM,SUBSUN;
ARRAY A,A1 [0:N+N1];                                                                 SC  13:   010
        M+N+N1;NCN+  N/(N*N1);                                                       SC  13:   010
              X+(2+M)*(N+(N1+1))*(N1+(N+1));                                         SC  13:   312
        Y+(M+(M+2))*C;                                                               SC  13:   A12
        Z+GAMMA(N+L+1)*GAMMA(N-L1*GAMMA(N1+L1+1)* GAMMA(N1-L1));                     SC  13:  1511
A[0]+1;FOR T+1 STEP 1 WHILE T$N-1 DO                                                 SC  13:  1910
    A[T]+(-N/(2*T   ))*(N-L-T)*(N+L+1-T)*A[T-1];                                     SC  13:  2611
A1[0]+1;FOR T1+1 STEP 1 WHILE T1$N-1 DO                                              SC  13:  3210
    A1[T ]+(-N1/(2*T1   ))*(N1-L1-T1)*(N1+L1+1-T1]* A1[T1-1];                        SC  13:  3913
SUM+0; FOR T+0 STEP 1 WHILE T$N-1 DO                                                 SC  13:  4512
       BEGIN  SUBSUM+0; FOR T1+0 STEP 1 WHILE T1$N-1-T DO                            SC  13:  5311
              BEGIN SUBSUM+SUBSUM+A1[T1]*(NCN+T1)*GAMMA(M+2+T+T1) END;               SC  13:  5812
              SUM+SUM+A[T]*(NCN+T)*SUBSUM  END,                                      SC  13:  6A11
    BO+X*SUM / (Y*SQRT(Z));                                                          SC  13:  7111
END OF PROCEDURE BO;                                                                 SC  13:  7611
                                                                                     SC  13:  F910
REAL PROCEDURE I;                                                  13 IS   85 LONG, NEXT SEG     5
BEGIN                                                                                SC   5:  A010
REAL NUMI;                                                                           SC   5:  A010
                                                                                     SC   5:  6010
IF NSNTF THEN IF NSNTF THEN BEGIN                            START OF SEGMENT **********    14
I2+ IF NPOINTS[N]$NPOINTS[M] THEN NPOINTS[N] ELSE NPOINTS[M];                        SC  14:   010
NUMI+0;                                                                              SC  14:   212
FOR I1+1 STEP 1 UNTIL I2 DO                                                          SC  14:   611
   NUMI+NUMI+(1+(I1 MOD 2))*I1+A*RF[N,I1]*RF[M,I1]);                                 SC  14:   F10
I+  NORM(N)*NORM[M]*NUMI*NSTAN+5/0,75;                                               SC  14:   810
END ELSE I+BO(NEFF[N],L[N]),NEFF[M],L[M]),C);                                        SC  14:  1710
END OF PROCEDURE I;                                                                  SC  14:  2113
                                                                                     SC  14:  2711
PROCEDURE THOMASFERMI(K,N,L,NINT);                                 14 IS   30 LONG, NEXT SEG     5
VALUE K,N,L,NINT;                                                                    SC   5:  A010
REAL N;   INTEGER K,L,NINT;                                                          SC   5:  A010
BEGIN                                                                                SC   5:  6010
REAL NFM1,NFO,NFP1,NS0,NSP1,FACTORM1,FACTORO,FACTORP1,EPSILON,                       SC   5:  6010
                                                                                     SC   5:  6010
    N2,N2TA,N2012,N2TS00,T2TA,RMAX,INVR,SCALE,JUMP,NORMOD,RATIO,ORATIO;  START OF SEGMENT **********    15
INTEGER NEWI2,LPOLY,DIRECTION,OLDDIRECTION,NODES;                                    SC  15:   010
ARRAY GSWF[0:2501,A[0:20]];                                                          SC  15:   010
BOOLEAN BEFORE,LASTTIME,VARYSCALE,INSIDE;                                            SC  15:   010
LABEL REPEAT,QUIT;                                                                   SC  15:   312
VARYSCALE+ IF R=1 THEN TRUE ELSE FALSE;                                              SC  15:   312
EPSILON+-(C/N1+2);                                                                   SC  15:   312
LPOLY+10*L*1L+1)+S;                                                                  SC  15:   A11
A[0]+1;                                                                              SC  15:   811
                                                                                     SC  15:  1110
```

```
FOR I1←1 STEP 1 UNTIL N+L+1 DO
   A[I1]←-N/(2×I1)×(N+L-I1)×(N+L+1-I1)×A[I1-1];
RMAX←1+R/(N+1);
RMAX←N×(N+1)×(UMAX+LN(FMAX+LN(RMAX)))/C;
SCALE←1;
JUMP←0.05;
BEFORE←TRUE;
DIRECTION←0;
LASTTIME←NOT VARYSCALE;
INSIDE←FALSE;
NORMOD←0;
ORATIO←RATIO←1;
REPEAT:
IF JUMP<0.0005 OR ABS(ORATIO)≤0.01×RATIO THEN LASTTIME←TRUE;
SCALE←SCALE+DIRECTION×JUMP;
NODES←0;
H←HSTAN×SQRT(SCALE);
I2←SQRT(RMAX)/H;
INVP←((I2+1)×H)↑(-2);
WFP1←0;
FOR I1←ENTIER(N+L+1) STEP -1 UNTIL 0 DO
   WFP1←A[I1]+INVP×WFP1;
WFP1←EXP(-C/(H×INVP))×INVP×(-N+0.25)×WFP1;
INVR←((I2+2)×H)↑(-2);
WF0←0;
FOR I1←ENTIER(N+L+1) STEP -1 UNTIL 0 DO
   WF0 ←A[I1]+INVR×WF0;
WF0 ←EXP(-C/(H×INVR))×INVR↑(-N+0.25)×WF0;
H2TA←A×H↑2;
H2D12←H↑2/12;
H2TSQA←5×H↑2/6;
KSP1←LPOLY/(H2TA×(I2+1)↑2)+VMOD[2×I2+2]-H2TA×(I2+1)+2×EPSILON;
KS0 ←LPOLY/(H2TA×(I2+2)↑2)+VMOD(2×I2+4)-H2TA×(I2+2)+2×EPSILON;
FACTORP1←1-H2D12×KSP1;
FACTOR0 ←1-H2D12×KS0;
FOR I1←I2 STEP -1 UNTIL 1 DO BEGIN
   WFM1←WF0;
   WF0←WFP1;
   KS0←KSP1;
   FACTORM1←FACTOR0;
   FACTOR0←FACTORP1;
   Y2TA←H2TA×I1↑2;
   KSP1←LPOLY/Y2TA+VMOD[2×I1]-Y2TA×EPSILON;
   FACTORP1←1-H2D12×KSP1;
   WFP1←((2+H2TSQA×KS0)×WF0-FACTORM1×WFM1)/FACTORP1;



   IF SIGN(WFP1)≠SIGN(WF0) THEN NODES←NODES+1;
   IF LASTTIME THEN BEGIN
      NORMOD←NORMOD+(1+(I1 MOD 2))×(I1×WFP1)↑2;
      IF VARYSCALE THEN SSPF[I1]←WFP1 ELSE BEGIN
         WF[K,I1]←WFP1;
         IF SIGN(KSP1)=-1 THEN INSIDE←TRUE;
         IF INSIDE THEN IF KSP1≥0 THEN IF A×I1≤I2 THEN BEGIN
            FOR I3←I1-1 STEP -1 UNTIL 1 DO BEGIN
               WF[K,I3]←WFP1×(I3/I1)↑(2×L+1.5);
               NORMOD←NORMOD+(1+(I3 MOD 2))×(I3×WF[K,I3])↑2;
            END;
         GO TO QUIT;
         END;
      END;
   END;
END;
IF LASTTIME THEN GO TO QUIT;
OLDDIRECTION←DIRECTION;
DIRECTION← IF NODES≤NINT-L-1 THEN 1 ELSE -1;
IF NODES=NINT-L-1 THEN BEGIN
   RATIO←2+(2×L+1.5)×(L+1-Z×H2TA)/(L+1-Z×H2TA/A);
   ORATIO←RATIO-WF0/WFP1;
   DIRECTION←SIGN(ORATIO);
END;
IF BEFORE THEN
   IF ABS(DIRECTION-OLDDIRECTION)≤1.5 THEN GO TO REPEAT
   ELSE BEFORE←FALSE;
IF NOT BEFORE THEN JUMP←JUMP/2;
GO TO REPEAT;
QUIT:
IF VARYSCALE THEN BEGIN
   NEWI2←ENTIER(I2×H/HSTAN);
   FOR I1←1 STEP 1 UNTIL NEWI2 DO WF[K,I1]←LAG(I1×HSTAN,0,H,SSPF,I2);
   I2←NEWI2;
END;
NORM[K]←SQRT(0.75/(H↑3×NORMOD));
NPOINTS[K]←I2;
WRITE (PRINTER[DBL],FTF,R,N,SCALE,HSTAN);
FOR I1←1 STEP 1 UNTIL 10,15 STEP 5 UNTIL I2 DO
   WRITE (PRINTER,FWF,I1,WF[K,I1]);
WRITE (PRINTER,FNNN,NORM[K],NINT-L-1,NODES);
TIPEIT(PRINTER);
WRITE(PRINTER,FL);
END OF PROCEDURE THOMASFERMI;
                                                      15 IS  287 LONG, NEXT SEG    9
```

```
PROCEDURE DIAG;
BEGIN
REAL JUNK,SPORBPARAM,SPORBPARAMP,HOLDSUM,SUMSQUARES;
ARRAY SPORBMATRIX3D,SPORBMATRIXP3D[0:5,0:4,0:4],TRACE,TRACES[0:5,0:7],      START OF SEGMENT **********  16
    TCALC[0:9],ELECPARAM[0:6],M[0:6,0:4];
INTEGER NELEC,NPARAM,IPARAM,SIZE,I6;
INTEGER ARRAY ELECMATRIX3D[0:5,0:4,0:6];
REAL DERIVDM;
ARRAY ALPHS[0:6,0:7],VTEMP,V2D[0:6,0:4],DERIV[0:4,0:6];
INTEGER IPARAMV,IPARAMH;
INTEGER IT;
REAL BD,TH,CT;
LABEL ITTYPE2,ERROR,SKIM;
WRITE (PRINTER,FL1);
IF HOLD=0 THEN BEGIN NELEC←2; NPARAM←3;
END ELSE BEGIN NELEC←4; NPARAM←4; END;
FOR IJ←IJMIN STEP 1 UNTIL IJMAX DO BEGIN
    SIZE←I2MAX[HOLD,IJ];
    I6←IJ-IJMIN+1;
    FOR IPARAM←1 STEP 1 UNTIL NPARAM+1 DO TRACE[I6,IPARAM]←0;
    FOR I1←1 STEP 1 UNTIL IMAX[IJ] DO
        TRACE[I6,NPARAM+1]←TRACE[I6,NPARAM+1]+T2D[IJ,I1];
    FOR I2←1 STEP 1 UNTIL SIZE DO BEGIN
        FOR IELEC←1 STEP 1 UNTIL NELEC DO BEGIN
            ELECMATRIX3D[IJ,I2,IELEC]←ELECMATRIX4D[HOLD,IJ,I2,IELEC];
            TRACE[I6,IELEC]←TRACE[I6,IELEC]+ELECMATRIX3D[IJ,I2,IELEC];
        END;
        FOR I3←1 STEP 1 UNTIL SIZE DO BEGIN
            SPORBMATRIX3D[IJ,I2,I3]←SPORBMATRIX4D[HOLD,IJ,I2,I3];
            SPORBMATRIXP3D[IJ,I2,I3]←SPORBMATRIXP4D[HOLD,IJ,I2,I3];
        END;
        TRACE[I6,NELEC+1]←TRACE[I6,NELEC+1]+SPORBMATRIX3D[IJ,I2,I2];
        IF HOLD=0 THEN
        TRACE[I6,NELEC+2]←TRACE[I6,NELEC+2]+SPORBMATRIXP3D[IJ,I2,I2];
    END;
END;
IT←0;
TCALC[0]←-P2D;
IF HOLD=0 THEN BEGIN
    SNEB(TRACE,3,JUNK,6);
    IF JUNK=0 THEN WRITE (PRINTER[PAGE],FERROR);
    FOR IELEC←1,2 DO ELECPARAM[IELEC]←TRACE[IELEC,6];
    SPORBPARAM←TRACE[3,6];
END ELSE IF HOLD=1 THEN BEGIN


        FOR IJ←IJMIN STEP 1 UNTIL IJMAX DO BEGIN
            I6←IJ-IJMIN+1;
            FOR IELEC←1,2,3 DO TRACES[I6,IELEC]←TRACE[I6,IELEC];
            TRACES[I6,4]←TRACE[I6,5];
            TRACES[I6,5]←TRACE[I6,7];
        END;
        SNEB(TRACES,4,JUNK,5);
        IF JUNK=0 THEN WRITE (PRINTER[PAGE],FERROR);
        FOR IELEC←1,2,3 DO ELECPARAM[IELEC]←TRACES[IELEC,5];
        ELECPARAM[4]←0;
        SPORBPARAM←TRACES[4,5];
        SPORBPARAMP←0;
 END ELSE BEGIN
        FOR IJ←IJMIN STEP 1 UNTIL IJMAX DO BEGIN
            I6←IJ-IJMIN+1;
            FOR IELEC←1,2,3,4,5 DO TRACES[I6,IELEC]←TRACE[I6,IELEC];
            TRACES[I6,6]←TRACE[I6,7];
        END;
        SNEB(TRACES,5,JUNK,6);
        IF JUNK=0 THEN WRITE (PRINTER[PAGE],FERROR);
        FOR IELEC←1 STEP 1 UNTIL 4 DO ELECPARAM[IELEC]←TRACES[IELEC,6];
        SPORBPARAM←TRACES[5,6];
        SPORBPARAMP←0;
END;
ITTYPE2:
TIMEIT(PRINTER);
WRITE (PRINTER[DBL],FPARAM,FOR IELEC←1,2,3,4 DO ELECPARAM[IELEC],
    SPORBPARAM,SPORBPARAMP);
HOLDSUM←SUMSQUARES;
SUMSQUARES←0;
FOR IPARAMV←1 STEP 1 UNTIL NPARAM DO
FOR IPARAMH←1 STEP 1 UNTIL NPARAM+1 DO
    ALPHS[IPARAMV,IPARAMH]←0;
FOR IJ←IJMIN STEP 1 UNTIL IJMAX DO BEGIN
    SIZE←I2MAX[HOLD,IJ];
    FOR I2←1 STEP 1 UNTIL SIZE DO
    FOR I3←1 STEP 1 UNTIL SIZE DO
        M[I2,I3]←0;
    FOR I2←1 STEP 1 UNTIL SIZE DO BEGIN
        FOR IELEC←1 STEP 1 UNTIL NELEC DO
            M[I2,I2]←M[I2,I2]+ELECMATRIX3D[IJ,I2,IELEC]×ELECPARAM[IELEC];
        FOR I3←1 STEP 1 UNTIL SIZE DO
        M[I2,I3]←M[I2,I3]+SPORBMATRIX3D[IJ,I2,I3]×SPORBPARAM
            +SPORBMATRIXP3D[IJ,I2,I3]×SPORBPARAMP;
   END;
```

```
IF SIZE=1 THEN BEGIN
   TCALC[1]←W[1,1];
   V2D[1,1]←1;
   GO TO SKIP;
END;
FOR I2←1 STEP 1 UNTIL SIZE DO
FOR IA←1 STEP 1 UNTIL SIZE DO
   VTEMP[I2,IA]← IF I2=IA THEN 1 ELSE 0;
JACOBI(SIZE,W,VTEMP,R=F,RD, W,CT);
FOR IA←1 STEP 1 UNTIL SIZE DO BEGIN
   FOR I1←IA STEP -1 WHILE W[IA,IA]<TCALC[I1-1] DO BEGIN
      TCALC[I1]←TCALC[I1-1];
      FOR I2←1 STEP 1 UNTIL SIZE DO
         V2D[I2,I1]←V2D[I2,I1-1];
   END;
   TCALC[I1]←W[IA,IA];
   FOR I2←1 STEP 1 UNTIL SIZE DO
      V2D[I2,I1]←VTEMP[I2,IA];
END;
SKIP:
WRITE (PRINTER,F1J,LOWERBLOCK+1J);
FOR I1←1 STEP 1 UNTIL SIZE DO BEGIN
WRITE (PRINTER,FV,T2D[IJ,I1],TCALC[I1],FOR I2←1,2,3,4 DO V2D[I2,I1]);
   FOR I2←1 STEP 1 UNTIL SIZE DO
      V3D[LOWERBLOCK+1J,I1,I2]←V2D[I2,I1];
END;
FOR I1←1 STEP 1 UNTIL IMAX[IJ] DO BEGIN
   FOR IELEC←1 STEP 1 UNTIL NELEC DO BEGIN
      DERIVDD←0;
      FOR I2←1 STEP 1 UNTIL SIZE DO
         DERIVDD←DERIVDD+V2D[I2,I1]×ELECMATRIX3D[IJ,I2,IELEC]×
            V2D[I2,I1];
      DERIV[I1,IELEC]←DERIVDD;
   END;
   DERIVDD←0;
   FOR I2←1 STEP 1 UNTIL SIZE DO
   FOR I3←1 STEP 1 UNTIL SIZE DO
      DERIVDD←DERIVDD+V2D[I2,I1]×SPORRMATRIX3D[IJ,I2,I3]×V2D[I3,I1];
   DERIV[I1,NELEC+1]←DERIVDD;
   IF HOLD≠0 THEN BEGIN
      DERIVDD←0;
      FOR I2←1 STEP 1 UNTIL SIZE DO
      FOR I3←1 STEP 1 UNTIL SIZE DO
         DERIVDD←DERIVDD+V2D[I2,I1]×SPORBMATRIXP3D[IJ,I2,I3]×
            V2D[I3,I1];

      DERIV[I1,NELEC+2]←DERIVDD;
      END;
   END;
FOR I1←1 STEP 1 UNTIL SIZE DO
WRITE (PRINTER,FDERIV,FOR IPARAM←1 STEP 1 UNTIL 6 DO DERIV[I1,IPARAM]);
IF HOLD=0 THEN WRITE (PRINTER[DBL],FCHECK,0,0,0) ELSE
WRITE (PRINTER[DBL],FCHECK,BD,TP,CT);
   FOR I1←1 STEP 1 UNTIL IMAX[IJ] DO BEGIN
      SUMSQUARES←SUMSQUARES+(TCALC[I1]-T2D[IJ,I1])*2;
      FOR IPARAMV←1 STEP 1 UNTIL NPARAM DO BEGIN
         ALPHS[IPARAMV,NPARAM+1]←ALPHS[IPARAMV,NPARAM+1]
            -(TCALC[I1]-T2D[IJ,I1])×DERIV[I1,IPARAMV];
         FOR IPARAMH←1 STEP 1 UNTIL NPARAM DO
            ALPHS[IPARAMV,IPARAMH]←ALPHS[IPARAMV,IPARAMH]
            +DERIV[I1,IPARAMV]×DERIV[I1,IPARAMH];
      END;
   END;
END;
SHEQ(ALPHS,NPARAM,JUNK,NPARAM+1);
IF JUNK≠0 THEN WRITE (PRINTER[PAGE],FERROR);
FOR IELEC←1 STEP 1 UNTIL NELEC DO
   ELECPARAM[IELEC]←ELECPARAM[IELEC]+ALPHS[IELEC,NPARAM+1];
SPORRPARAM←SPORRPARAM+ALPHS[NELEC+1,NPARAM+1];
IF HOLD≠0 THEN
SPORBPARAMP←SPORBPARAMP+ALPHS[NELEC+2,NPARAM+1];
IT←IT+1;
WRITE (PRINTER[DBL],FSUM,SUMSQUARES,IT);
WRITE (PRINTER,FL);
IF ABS(HOLDSUM-SUMSQUARES)≥SUMSQUARES×R-3 THEN GO TO ITTYPE2;
ERROR:
END OF PROCEDURE DIAG;
                                              10 IS  547 LONG, NEXT SEG    5
TIMEIT(PRINTER);
READ (READER /,NMAX,NNMAX);
READ (READER,/,ONEFF);
READ (READF1,/,Z,NEL,C);
WRITE (PRINTER[DBL],F1,Z,NEL,C,NMAX,ONEFF);
WRITE (READF2,F2,Z,NEL,C,NMAX,ONEFF);
C1←0.587234;
FOR N←1 STEP 1 UNTIL NMAX DO
READ (READF1,/,N,NEFF[N],CORE[N],L[N],K[N],J[N],T[N]);
REWIND(READF1) ;
LOCK(READF1) ;
FOR N←1 STEP 1 UNTIL 31 DO NINT[N]←
   IF N≤5 THEN A+L[N]
```

```
   ELSE Y←L[N];
FOR I1←0 STEP 1 UNTIL 15 DO
READ (READER,/,I2,AA[I2],BB[I2],CC[I2]);
IF C/Z≤0,1 THEN BEGIN
   QQ←LN(C/Z);
   QQSUM←0;
   FOR I1←10 STEP -1 UNTIL 0 DO
      QQSUM←CC[I1]+QQSUM×QQ;
   X0←EXP(QQSUM);
END [illegible] /Z≤0,5 THEN BEGIN
   QQ←LN(C/Z);
   QQSUM←0;
   FOR I1←12 STE[illegible] -1 UNTIL 0 DO
      QQSUM←BB[I1]+QQSUM×QQ;
   X0←QQSUM;
END ELSE BEGIN
   QQ←(1-C/Z)↑(2/3);
   QQSUM←0;
   FOR I1←15 STEP -1 UNTIL 0 DO
      QQSUM←AA[I1]+QQSUM×QQ;
   X0←QQSUM;
END;
M←X0/4096;
M32←M↑1.5;
I2←64;
PHIP1←0;
PHI0←-C/(4096×Z);
FOR I1←4096 STEP -1 UNTIL 1 DO BEGIN
   PHIM1←PHI0;
   PHI0←PHIP1;
   PHIP1←PHI0×(2+M32×SQRT(PHI0/I1))-PHIM1;
   IF I1=I2×2 THEN BEGIN
      VMOD[I2]←-I1×C/512-B×Z×PHI0;
      I2←I2-1;
   END;
END;
FOR I2←65 STEP 1 UNTIL 500 DO VMOD[I2]←-A×C;
   MSTAR←SQRT(0.8853×Z↑(-1/3)×X0)/32;
TIMEIT(PRINTER);
WRITE (PRINTER,FL);
FOR N←1 STEP 1 WHILE NEFF[N]=NEFF[1]≤NEFF DO
   THOMASFERMI(N,NEFF[N],L[N],NINTEN);
NTF←N-1;
FOR MOLD←0 STEP 1 UNTIL 3 DO BEGIN
READ (READER,/,LM1,LSAME,LP1,LM150,LP150);


FOR J2←MOLD-2 STEP 1 UNTIL MOLD+[illegible] DO IF J2>0 THEN BEGIN
   I2←0;
   FOR S2←0,1 DO
   FOR L2←ABS(J2-S2) STEP 1 UNTIL J2+S2 DO
   IF L2≥ABS(MOLD-1) AND L2≤MOLD+1 THEN BEGIN
      I2←I2+1;
      ELECMATRIXAO[MOLD,J2,I2,1]←1;
      IF MOLD=0 THEN    ELECMATRIXAO[0,J2,I2,2]← IF S2=0 THEN 1 ELSE -1
      ELSE BEGIN
         IF L2=MOLD-1 THEN BEGIN
            ELECMATRIXAO[MOLD,J2,I2,2]←LM1;
            ELECMATRIXAO[MOLD,J2,I2,3]← IF S2=0 THEN LM150 ELSE 0;
            ELECMATRIXAO[MOLD,J2,I2,4]←0;
         END ELSE IF L2=MOLD THEN BEGIN
            ELECMATRIXAO[MOLD,J2,I2,2]←LSAME;
            ELECMATRIXAO[MOLD,J2,I2,3]←0;
            ELECMATRIXAO[MOLD,J2,I2,4]← [illegible];
         END ELSE BEGIN
            ELECMATRIXAO[MOLD,J2,I2,2]←LP1;
            ELECMATRIXAO[MOLD,J2,I2,3]←0;
            ELECMATRIXAO[MOLD,J2,I2,4]← IF S2=0 THEN LP150 ELSE 0;
         END; END;
         I3←0;
         FOR S3←0,1 DO
         FOR L3←ABS(J2-S3) STEP 1 UNTIL J2+S3 DO
         IF L3≥ABS(MOLD-1) AND L3≤MOLD+1 THEN BEGIN
            I3←I3+1;
            IF ABS(L3-L2)≤1 AND L2+L3≠0 THEN BEGIN
            SP←W2MOD(1,L2,1,L3,MOLD);
            SPP←W2MOD(MOLD,L2,MOLD,L3,1);
            G←-W2MOD(S2,L2,S3,L3,J2)/[illegible];
            IF L3=L2+1 THEN G←G×L3×(2×L2+1) ELSE
            IF L3=L2 THEN G←G×L2×(L2+1) ELSE
            G←G×L2×(2×L2+1);
            SP←SQRT(SP×G)/2;
            SPP←SQRT(SPP×G[illegible]
            IF S2-S3≠0 THEN SP←-SP;
            IF L2-L3≠0 THEN SPP←-SPP;
            IF S2≠S3 AND S2-S3=L3-L2 THEN BEGIN SP←-SP; SPP←-SPP; END;
            IF L2=L3 AND L2×(L2+1)+2≤MOLD×(MOLD+1) THEN SP←-SP;
            IF L2=L3 AND L2×(L2+1)+MOLD×(MOLD+1)≤2 THEN SPP←-SPP;
            IF L2=L3 AND S2=S3 AND [illegible]+1)≤L2×(L2+1)+S2×(S2+1) THEN
               BEGIN SP←-SP; SPP←-SPP; END;
         END ELSE BEGIN SP←0; SPP←0; END;
         SPORBMATRIXAO[MOLD,J2,I2,I3]←-SP;
```

```
          SPORBMATRIXPAU[HOLD,J2,I2,I3]+SPP;
ENDI
ENDI
   I2MAX[HOLD,J2]+I2;
ENDI
ENDI
FOR LGREATER+1 STEP 1 UNTIL 3 DO BEGIN
   I2+0;
FOR J2+LGREATER-3 STEP 1 UNTIL LGREATER+1 DO
IF J2≥0 THEN BEGIN
   I2LOWER[LGREATER-1,J2]+I2;
FOR S2+0,1 DO
FOR L2+ABS(J2-S2) STEP 1 UNTIL J2+ S2 DO
IF L2≥ABS(LGREATER-2) AND L2≤LGREATER THEN BEGIN
   I3+0; I2+I2+1;
FOR J3+LGREATER-2 STEP 1 UNTIL LGREATER+2 DO
IF J3≥0 THEN BEGIN
   I3LOWER[LGREATER,J3]+I3;
FOR S3+0,1 DO
FOR L3+ABS(J3-S3) STEP 1 UNTIL J3+S3 DO
IF L3≥ABS(LGREATER-1) AND L3≤LGREATER+1 THEN BEGIN
   I3+I3+1;
   IF ABS(J2-J3)≤1 AND ABS(L2-L3)≤1 AND (J2+J3)≠0 AND S2=S3 THEN BEGIN
      STLS+SQRT((2×J2+1)×
                 W2=OD(L2,J2,L3,J3,S2)×W2=OD(LGREATER-1,L2,LGREATER,L3,1)/
               X[(L2,L3)]);
      IF   J=L2+J2-J3=1 THEN STLS+-STLS;
      IF L3=L2 THEN STLS+-STLS;
      END ELSE STLS+0;
      STLS30[LGREATER,I2,I3]+STLS;
END; END; END; END; END;
WRITE(PRINTER,FL);
LOWERBLOCK+0; HOLD+-1; IJMAX+0; IJMIN+10;
FOR IJ+0 STEP 1 UNTIL 10 DO T20[IJ,0]+-1;
FOR N+2 STEP 1 UNTIL NMAX+1 DO BEGIN
   IF HOLD≠L[N] THEN BEGIN
      FOR IJ+IJMIN STEP 1 UNTIL IJMAX DO
      FOR I1+1 STEP 1 UNTIL IMAX[IJ] DO
         INDEX[N20[IJ,I1]]+I1;
      IF HOLD≠-1 THEN DIAG;
      LOWERBLOCK+LOWERBLOCK+IJMAX+1;
      IJMAX+0;  IJMIN+10;
      FOR IJ+0 STEP 1 UNTIL 10 DO IMAX[IJ]+0;
   END;
   IJ+ENTIER(J[N]);

   IF IJ≥IJMAX THEN IJMAX+IJ;
   IF IJ≤IJMIN THEN IJMIN+IJ;
   BLOCK[N]+LOWERBLOCK+IJ;
   IMAX[IJ]+IMAX[IJ]+1;
   FOR I1+IMAX[IJ] STEP -1 WHILE T[N]≤T20[IJ,I1-1] DO BEGIN
      T20[IJ,I1]+T20[IJ,I1-1];
      N20[IJ,I1]+N20[IJ,I1-1];
   END;
   T20[IJ,I1]+T[N];
   N20[IJ,I1]+N;
   HOLD+L[N];
END;
WRITE (PRINTER,FL);
BLOCK[1]+0; INDEX[1]+1;
V30[0,1,1]+SQRT(6);    V30[0,1,2]+0;
FOR N+1 STEP 1 UNTIL  NNMAX
DO BEGIN  SUM1+0;SUM2+0;SUM3+0;  WRITE (PRINTER[DBL],FA);
SIZE2+I2MAX[L[N],ENTIER(J[N])];
I2LOWER00+I2LOWER[L[N],J[N]];
FOR I2+1 STEP 1 UNTIL SIZE2 DO
   V10[I2]+V30[BLOCK[N],INDEX[N],I2];
FOR M+1 STEP 1 UNTIL NMAX DO
IF ABS(L[M]-L[N])=1 AND ABS(J[M]-J[N])≤1  AND (J[N] + J[M])≠0
AND ABS(NEFF[M]-NEFF[N])≤DNEFF
THEN BEGIN
   LGREATER+MAX(L[M],L[N]);
   SIZE3+I2MAX[L[M],ENTIER(J[M])];
   I3LOWER00+I3LOWER[L[M],J[M]];
   OS+0;
   IF L[M]=LGREATER THEN
      FOR I2+1 STEP 1 UNTIL SIZE2 DO
      FOR I3+1 STEP 1 UNTIL SIZE3 DO
         OS+OS+V10[I2]×STLS30[LGREATER,I2+I2LOWER00,I3+I3LOWER00]×
            V30[BLOCK[M],INDEX[M],I3]
   ELSE
      FOR I3+1 STEP 1 UNTIL SIZE3 DO
      FOR I2+1 STEP 1 UNTIL SIZE2 DO
         OS+OS+V10[I2]×STLS30[LGREATER,I3+I3LOWER00,I2+I2LOWER00]×
            V30[BLOCK[M],INDEX[M],I3];
   OS+(OS×1)↑2/((4×LGREATER↑2-1)×(2×J[N]+1));
 TT+T[M]-T[N];    YY+C[×TT];     SUM1+SUM1+OS;      SUM2+SUM2+OS/TT;
 LAMBDA+@8/,TT;         SUM3+SUM3 + OS×TT;
A+2.02605@-1×OS×TT↑3;
A+A×(2×J[N]+1)/(2×J[M]+1);
WRITE (PRINTER,FS,N,M,OS,YY,LAMBDA,A);
```

```
      WRITE (READF2,F0,N,M,DS,YY));                                                         SC    51 70011
      END;                                                                                  SC    51 72111
      WRITE (PRINTER[DBL],F3,N,SUM1,SUM2,SUM3));                                            SC    51 72512
      WRITE (READF2,F4,N,N,SUM1,SUM2));                                                     SC    51 73911
      TIMEIT(PRINTER));                                                                     SC    51 75311
      WRITE (READF2,F7,N,COREIN],L[N],K[N],J[N],T[N]));                                     SC    51 75A11
      END ; REWIND(READF2) ; END ;                                                          SC    51 77211
                                                                            5 IS   760 LONG, NEXT SEG    2
      LOCK (READF2));                                                                       SC    21  1210
      END,                                                                                  SC    21  1313
                                                                            2 IS    17 LONG, NEXT SEG    1
    EXP              IS SEGMENT NUMBER 0017, PRT ADDRESS IS 0207
    LN                                 0018                 0206
    SQRT                               0019                 0076
    OUTPUT(W)                          0020                 0082
    BLOCK CONTROL                      0021                 0005
    INPUT(W)                           0022                 0094
    X TO THE I                         0023                 0216
    GO TO SOLVER                       002A                 0075
    ALGOL WRITE                        0025                 001A
    ALGOL READ                         0026                 0015
    ALGOL SELECT                       0027                 0016
NUMBER OF ERRORS DETECTED =    0                          LAST CARD WITH ERROR HAS SEQ #
PRT SIZE = 200; TOTAL PGM SEGM SIZE =  2600 WORDS; DISK SIZE = 160 SEGS; NO, PGM, SEGS =  28
ESTIMATED CORE STORAGE REQUIREMENT =  7025 WORDS,
13:19:37 WEDNESDAY, MAY 10, 1967    PROCESSOR TIME = 55,A2 SECONDS    I/O TIME = 59,87 SECONDS



LABEL  000000000LINE   00167150Y  COMPILE GIANT/FIASCO  SYNTAX                                  ORO7PACC ALGOL
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APPENDIX C

CALCULATION OF THE OPTICAL RADIATION EMITTED BY A CYLINDRICAL ARC OF KNOWN TEMPERATURE PROFILE

by. R. Liebermann

INTRODUCTION

In order to compare measurable physical properties of an emitting plasma with theory, a computer program has been written to calculate at the surface of a cylindrical arc discharge:

(1) the spectral radiance (normal to the surface) due to radiant contribution from along the line of sight of the diameter which has a spatial temperature gradient, and

(2) the spectral radiant emittance due to contributions from all radiating volume elements of a homogeneous temperature arc column.

The above calculations involve self-absorption processes within the arc column and therefore are solutions of a radiant heat transfer equation.

A. Radiant Heat Transfer Equation

With the assumption that the plasma is in local thermal equilibrium (LTE) the spectral radiance is related to the properties of the medium through the radiant heat transfer equation

$$-\frac{d I_\nu}{d \tau_\nu} = I_\nu - B_\nu \qquad (1)$$

which describes the spatial gradient of intensity along the line of sight at some point x where I_ν is the spectral radiant intensity at frequency ν in the proper direction, B_ν is the corresponding black body intensity and τ_ν is the optical depth as measured from $x = -\infty$ to x. We define the optical depth as

$$\tau_\nu(T) \equiv \int_{-\infty}^{x} \kappa'_\nu \ (T)\ ds \qquad (2)$$

where κ'_ν (T) is the spectral absorptivity coefficient (including stimulated emission) due to free-free, bound-free, and bound-bound radiative processes. The solution of 1 is given as

$$I_\nu(\bar{\tau}_\nu) = \int_0^{\bar{\tau}_\nu} B_\nu(\tau_\nu)\ \exp\{-\bar{\tau}_\nu + \tau_\nu\}\ d\nu \qquad (3)$$

where

$$\bar{\tau}_\nu \equiv \int_{-\infty}^{L} \kappa'_\nu\ (T)\ ds \qquad (4)$$

with L corresponding to that location along the line of sight (at the surface of the arc column) having spectral radiance $I_\nu(\bar{\tau}_\nu)$. In 3 it was assumed for $x \leq 0$ that no contribution to $I_\nu(\bar{\tau}_\nu)$ is made (i.e., no external radiation field is present).

1. Spectral Radiance

If our interest is radiance at the arc column's surface due to contributions from along the line of sight of the diameter, equation 3 by an assumption of radial symmetry can be placed in the following form.

$$I_\nu(\bar{\tau}_\nu) = I_\nu(r=R) = \int_0^{\bar{Z}} B_\nu(Z) \left[\exp\{Z\} + \exp\{-Z\} \right] \exp\{-\bar{Z}\}\ dZ \qquad (5)$$

where Z is an optical depth measured from the center of the arc column to some radial point r along the radius which has a maximum dimension R. The correspondence is Z = o at r = o and Z = $\bar{Z}$ at r = R thus

$$\bar{Z} = \int_o^R \kappa'_\nu (T(r))\, dr \; ; \; Z = \int_o^r \kappa'_\nu (T(r))\, dr \qquad (6)$$

For programming purposes Equation 5 is the better form of 3. In order to solve 5 it is first necessary to have prior knowledge of the temperature profile T(r) and for a given gas vapor pressure a method by which κ'_ν can be determined such that solutions of 6 are obtainable. Part D of this section describes the general theory involved for determining $\kappa'_\nu(T)$.

Utilizing the theory of Part D we are then prepared to numerically integrate Equations 6 and thus 5. The method of approach was as follows. For a specified temperature profile and frequency the integrand of 6 was determined at division points in r and interpolated in r^2 between division points. Using a linear expansion of κ'_ν in r^2 a closed form integration was performed between division points and a summation yielded Z(r). In similar fashion the black body term in the integrand of 5 was calculated at division points in r and linearly expanded in Z^2. A closed form integration of 5 was then possible between division points of Z(r) and was summed to yield $I_\nu(\bar{\tau}_\nu)$. Although the latter integration can be performed for all values of the parameters serious errors (due to cancellation effects) may develop when ΔZ is small between end points of the intervals. Hence for $\Delta Z < .01$ the solution was expanded in terms of ΔZ whereas for $\Delta Z > .01$ the closed form was used. Solution of 5 was then repeated for other selected ν values of the specified band pass to yield a representative spectrum.

2. Spectral Radiant Emittance

If our interest is spectral emittance at the arc column's surface due to contributions from all radiating volume elements with the

discherge assumed homogeneous in temperature then Equation 3 which yields the spectral radiance along a particular line of sight reduces to

$$I_\nu(T,S) = B_\nu(T) \left[1 - \exp\{ - \bar{\tau}_\nu \}\right] \qquad (7)$$

where now from Equation 4

$$\bar{\tau}_\nu = K'_\nu (T)\, S \qquad (8)$$

S being the distance through which radiation travels along a particular line of sight and is a function of arc geometry.

The spectral radiant emittance at the surface of the arc column can be calculated using 7 by applying the cosine law and integrating over solid angle. Using the geometry shown in Reference 1 the spectral radiant emittance is given as

$$F_\nu(T) = B_\nu(T) \left[\pi - 4 \int_0^{\pi/2} \int_0^1 \exp\left\{ \frac{- K'(T)\, D\, u}{u^2 + (1-u^2)\, \sin^2\phi} \right\} u\, du\, d\phi \right] \qquad (9)$$

where D is the column diameter

The radiant emittance is then determined by

$$F(T) = \int_0^\infty F_\nu(T)\, d\nu \qquad (10)$$

Equations (9) and (10) were solved using straightforward numerical techniques.

B. Input to Arc Intensity Program

The input required for the above calculations is fully described within the program itself which is shown in Part E of this Section. In brief the basic required input is as follows:

(1) Spectroscopic data involving bound-bound transitions such as

(a) oscillator strengths
(b) electron impact line shifts and widths
(c) excitation energies
(d) statistical weights

(2) thermodynamic properties such as tables of

(a) electron number densities
(b) neutral particle number densities
(c) internal partition functions
(d) ionization lowering values

(3) temperature profile

(4) specified wavelength band pass.

C. Output of Arc Intensity Program

The output of the program provides plots as well as printouts of the spectral radiance and spectral radiant emittance. In addition plots of spectral absorptivities are obtainable. Samples of these plots are shown in Figures 3, 4, and 5. For particulars on how to obtain these plots see program Part E.

D. Spectral Absorptivities

The net absorption coefficient κ' which is the difference between true absorption and induced emission coefficients is in a spectral line for a given frequency ν and temperature T (assuming LTE)

$$\kappa'_\nu(T) = \pi r_o c f_{mn} N_n \left[1-\exp\left\{\frac{-h\nu}{kT}\right\}\right] L(\nu) \qquad (11)$$

where π, r_o, c, h and k are the usual constants, f_{mn} is the absorption oscillator strength for transitions from state n to m (n being the lower energy level state), N_n is the population density of the initial state, and $L(\nu)$ is the line profile normalized such that

$$\int_{-\infty}^{\infty} L(\nu)d\nu = 1 \tag{12}$$

where $L(\nu)$ is a function of the lines, shifts, widths etc. all a function of temperature and pressure.

For conditions of LTE the population density N_n can be expressed in terms of N_o (the total number of atoms or ions in question) by use of the Boltzmann relation

$$N_n = \frac{g_n N_o}{U_o} \exp\left\{\frac{-E_n}{kT}\right\} \tag{13}$$

where g_n is the statistical weight of the initial level, E_n is the excitation energy of the initial level, U_o is the atomic (or ionic) internal partition function and T is the absolute electron temperature.

The line profile $L(\nu)$ is course dependent on the mechanisms of line broadening. The stark effect due to electron impact has the Lorentz dispersion profile given as

$$L(\nu) = \frac{1}{\pi\omega}\left[\frac{1}{\left[\frac{\nu-(\nu_o+d)}{\omega}\right]^2 + 1}\right] \tag{14}$$

where ω is the half width of the line at half intensity and d is the electron impact shift. ν_o is the observed frequency of the line in an unperturbed condition.

When resonance broadening mechanisms are of importance, one must add to the electron impact half width ω the resonance half width ω_R which from first order approximation can be expressed for resonance lines as

$$\omega_R = \frac{3r_o c}{4\pi}\left(\frac{g_1}{g_2}\right)^{1/2} \frac{f\ N_g}{\nu_o} \qquad (15)$$

where g_1 and g_2 are respectively the lower and upper states' statistical weight factors of the resonance line, N_g is the ground state population density and f is the absorption oscillator strength of the transition (actually f as defined here is the average value for the resonance multiplet transition obtained by a sum of the multiplet's individual f's over final states which are then averaged over initial states). In equation 15, N_g are neutral perturbers of the same kind (radiating atoms). For the case when perturbers of unlike kind are of such abundance (e.g. a strong concentration of another gas specie is present) then Van der Waals broadening may be of some importance and should be included in the dispersion profile.

Besides line broadening due to charge perturbers (Stark effect) or neutral atoms (Resonance and Van der Waals effects) there exists other broadening mechanisms which must also be considered, namely Doppler broadening, which results in a Gaussian line shape profile. This type of profile is dominant when collisions are negligible and the velocities of the radiating systems have a thermal distribution. The Gaussian line shape is given as

$$L_D(\Delta\nu) = \left(\frac{\ell n 2}{\pi}\right)^{1/2} \frac{1}{\omega_o} \exp\left[\frac{-\ell n 2}{\omega_D^2}(\Delta\nu)^2\right] \qquad (16)$$

with $\Delta\nu = \nu - \nu_o$ and where ω_D is the Doppler half (half) width

$$\omega_D = \left[\frac{2kT\ell n 2}{Mc2}\right]^{1/2} \nu_o \qquad (17)$$

M being the mass of the radiating system. When collision effects cannot be neglected (e.g. when ω, ω_R etc. are of the same order of magnitude as ω_D) then joint effects of Doppler and the more important pressure

broadening mechanisms should be considered. The observed line shape is then the so called Voigt profile provided the broadening processes are statistically independent. From 17 it is obvious that lines occurring in the UV regions will tend to be more of a Voigt profile type.

The net absorption coefficient κ'_ν as expressed in 6 is not only due to bound-bound transitions but also includes bound-free and free-free processes as well. Therefore, one must add to a sum of Equation 11 these other processes to obtain representative values of 5 in the spectral regions where bound-bound transitions are not dominant. For conditions of LTE the bound free absorptivity $\kappa_{bf}(\nu,T)$ can be expressed in terms of a sum over excited states designated by quantum numbers n and ℓ having corresponding photoionization cross-sections $\sigma_{n\ell}$ and population density $N_{n,\ell}$ whose edge frequencies $\nu_{n\ell}$ are less than or equal to ν

$$\kappa_{bf}(\nu,T) = \left.\sum_{n,\ell} \sigma_{n\ell} N_{n\ell}\right\}_{\nu_{n\ell}\leq\nu} \qquad (18)$$

The net bound-free absorptivity is then expressed as

$$\kappa'_{bf}(\nu,T) = \kappa_{bf}(\nu,T)\left[1 - \exp\left\{\frac{-h\nu}{kT}\right\}\right] \qquad (19)$$

Solution of 18 is a formidable task since $\sigma_{n\ell}$ for each level requires numerical solutions of the Schrodinger equation.* A simplified approach is to separate 18 into two distinctive regions i.e., into levels which are hydrogen like and into levels which are non hydrogen like thus

$$\kappa_{bf}(\nu,T) = \sum_{n,\ell} \sigma_{n_\ell} N_{n_\ell} + \sum_{n,\ell} \sigma^{H}_{n_\ell} N^{H}_{n_\ell} \qquad (20)$$

*See for example Ref. 1.

where in general for the hydrogen like terms n>>1. The sum over the hydrogenic levels can be simplified further as follows. Starting with a sum rule analogous to that for bound-bound transitions

$$\int_{\nu_{n\ell}}^{\infty} \sigma_{n\ell}^{H} d\nu = \pi r_o c f_{n\ell} \tag{21}$$

and using the proportionality $\sigma_{n\ell}^{H} \sim \nu^{-3}$ the hydrogenic photoionization cross section $\sigma_{n\ell}^{H}$ is

$$\sigma_{n\ell}^{H} = 2\pi r_o c \frac{\nu_{n\ell}^2}{\nu^3} f_{n\ell} \tag{22}$$

where $f_{n\ell}$ corresponds to the excited n,ℓ state's continuum oscillator strength. Using the Rydberg formula for hydrogenic energy levels, the binding energy E_B of the excited level is ($E_{n\ell} \simeq E_n$)

$$E_B = h\nu_{n\ell} = E_\infty - E_{n\ell} = \frac{E_H Z^2}{n^2} \tag{23}$$

where Z refers to the ionization stage, n is the principal quantum number, E_∞ is the ionization potential, $E_{n\ell}$ is the excitation energy of the excited level and E_H is the Rydberg constant. From 23 we see that the rate at which the binding energy changes with respect to unit change in principal quantum number for n>>1 is

$$\Delta E_B \simeq \frac{-2E_H Z^2}{n^3} \tag{24}$$

We now define an average hydrogenic cross section σ_n for all ℓ states with same quantum number n as

$$\sigma_n \equiv \sum_{\ell} (2\ell+1)\ \sigma^H_{n\ell} \Big/ \sum_{\ell} (2\ell+1) \qquad (25)$$

where ℓ is the orbital-angular momentum quantum number. Thus using the hydrogenic relations

$$\left.\begin{aligned} &\sum_{\ell} (2\ell+1) f_{n\ell} \simeq .5n \\ \text{and}\quad &\sum_{\ell} (2\ell+1) \Big|_{n=\text{constant}} = n^2 \end{aligned}\right\} \qquad (26)$$

Equation 25 takes the form of

$$\sigma_n = 4\pi^2 \frac{\alpha a_o^2}{n^5} \left(\frac{n}{h\nu}\right)^3 Z^4 \qquad (27)$$

where α and a_o are the usual constants. Equation 25 is the familiar hydrogenic cross section less the Gaunt factor G_{bf}. Using Equation 13, and noting for atomic gases, whose higher levels are hydrogen like but degenerate in J (total angular momentum quantum number) that

$$g_n = \sum (2J+1)_n = 2n^2 g_1 \qquad (28)$$

where g_1 is the statistical weight factor of the ground state of the parent term; and using the relationship of Equation 24 the hydrogenic sum term of 20 becomes

$$\sum_{n,\ell} \sigma^H_{n\ell} N^H_{n\ell} = \frac{-4\pi^2 \alpha a_o^2 g_1}{U_o E_H} \left(\frac{E_H}{h\nu}\right)^3 Z^2 N_o \sum \exp\left\{\frac{-E_n}{kT}\right\} \Delta E_B \cdot G_{bf} \qquad (29)$$

For hydrogen the excitation energy E_n is approximately equivalent to $E_{n\ell}$. However, for other gases whose higher levels are hydrogen like but degenerate in J then E_n should be averaged over these J,ℓ states which have $E_{J\ell}$ excitation energies such as

$$E_n = \sum_J (2J+1)_n \, E_{J\ell} / 2n^2 g_1 \qquad (30)$$

Thus with E_n as defined in 30 obeying Equation 23 wherein $E_{n\ell}$ is replaced by E_n then 29 takes the form of

$$\sum_{n\ell} \sigma^H_{n\ell} N^H_{n\ell} = \frac{-4\pi^2 \alpha a_o^2 g_1}{U_o E_F} \left\{\frac{E_H}{h\nu}\right\}^3 Z^2 N_o \, G_{bf} \, \exp\left\{\frac{-E^\infty}{kT}\right\} \cdot$$

$$\sum \exp\left\{\frac{E_B}{kT}\right\} \Delta E_B \qquad (31)$$

with the assumption that G_{bf} ≈ constant for n >>1.

The sum on the right of 31 may for practical purposes be taken as an integral with lower limit $E_B = h\bar{\nu}_n$ and upper limit E_B=o. Hence for $\bar{\nu}_n$ representing the maximum edge frequency of the merged levels where n>>1 with $\bar{\nu}_n \leq \nu$ then

$$\sum_{n\ell} \sigma^H_{n\ell} N^H_{n\ell} = \frac{4\pi^2 \alpha a_o^2 g_1}{U_o} \left(\frac{kT}{E_H}\right) Z^2 N_o \left(\frac{E_H}{h\nu}\right)^3 \exp\left\{\frac{-E^\infty}{kT}\right\} \left[\exp \left\{\frac{h\bar{\nu}_n}{kT}\right\} - 1\right] G_{bf} \qquad (32)$$

$$= 1.82 \times 10^{24} \frac{g_1 T}{U_o} Z^2 \frac{N_o}{\nu^3} \exp\left\{\frac{-E^\infty}{kT}\right\} \left[\exp\left\{\frac{h\bar{\nu}_n}{kT}\right\} - 1\right] G_{bf}$$

or for the case when ν is less then the maximum edge frequency of the merged levels ($\nu < \bar{\nu}_n$) then

$$\sum_{n\ell} \sigma^{H}_{n\ell} N_{n\ell} = 1.82 \times 10^{24} \frac{g_1 T}{U} Z^2 \frac{N_o}{\nu^3} \exp\left\{\frac{-E_\infty}{kT}\right\} \left[\exp\left\{\frac{h\nu}{kT}\right\} - 1\right] G_{bf} \qquad (33)$$

Equations 32 and 33 are equivalent to those presented by Biberman, Norman and Ulyanov[2] less their correction factor which for our high n levels is approximately one and equivalent to the Gaunt factor. It is of interest to note that in the form of 31 if the right hand sum is taken as an integral with lower limit set to E_B=o and upper limit E_B= - ∞ representing unbound electrons we obtain at once the familiar free-free absorptivity expression

$$\kappa_{ff} = 1.82 \times 10^{24} \frac{g_1 \, T \, N_o Z^2}{U_o \nu^3} \exp\left\{\frac{-E_\infty}{kT}\right\} \cdot G_{ff} \qquad (34)$$

where the G_{ff} term has been introduced and is the free-free Gaunt factor. Thus equation 20 takes the form (including the f-f absorption)

$$\kappa_{bf+ff} = \sum \sigma_{n\ell} N_{n\ell} + 1.82 \text{ s } 10^{24} \frac{g_1 \, T \, N_o Z^2}{U_o \nu^3} \exp\left\{\frac{-E_\infty}{kT}\right\} \cdot \left[G_{ff} + G_{bf} \left(\exp\left\{\frac{h\nu'}{kT}\right\} - 1\right)\right] \qquad (35)$$

whereby previous definitions $\nu' = \bar{\nu}_n$ if $\nu \geq \bar{\nu}_n$ and $\nu' = \nu$ if $\nu < \bar{\nu}_n$. In equation 35 the non-hydrogenic sum term then only includes such levels having edge frequencies ν_E which meet the requirement that $\bar{\nu}_n < \nu_E \leq \nu$. In the above derivations the assumption that G_{ff} is constant independent on temperature and frequency is valid provided T < 2 ev (see Ref. 3) however when T is of greater value than G_{ff} increases and varies somewhat with frequency. Likewise when n is of some lower value then G_{bf} is no longer a constant but varies with

quantum number and frequency. The accuracy of 35 is thus better enhanced when the sum term includes the majority of the excited levels. Such calculations involving the sum term have been made by Ref. 2 and [4] who have utilized the techniques proposed by Ref. 1 for determining photoionization cross sections for ionized gases other than hydrogens. However their results differ somewhat in that they have chosen different normalization factors. In essence (using their results) Equation 35 remains the same with the exception of replacing the factor $Z^2 G_{bf}$ with a ζ (Zeta) factor, and in addition when using the ζ factor of Ref. [4], ν' is to be replaced by ν for all values. Their sum term then only includes a limited number of lower excited levels (including the ground state).

Since several b-b transitions usually occur for a given lower excited state near the frequency of its continuum photoionization edge (the upper excited state being near the ionization limit) there results a pseudo continuum (i.e. the lines in question merge with the continuum causing in appearance a false photoionization edge at a slightly lower frequency). When these b-b transitions are not included in the sum of Equation 11 near such corresponding photoionization edges then serious errors may develop in solutions of radiant heat transfer problems. Therefore in order to avoid such difficulty (when all such b-b transitions are not fully resolved) one should assign a correction term to the photoionization edge ν_E to yield an apparent edge ν'_E such as

$$\nu'_E = \nu_E - \Delta E_S/h \qquad (36)$$

where h is the usual constant and ΔE_S is the so called advance of the series limit (see Ref. [5]), and let the photoionization edge cross-section $\sigma(\nu_E)$ for this particular level be defined at ν'_E. In addition the lowering of the ionization potential ΔE_∞ should be included in the calculation of ν_E such as

$$h\nu_E = E_\infty - \Delta E_\infty - E_{n\ell} \qquad (37)$$

where E_∞ is the ionization potential and $E_{n\ell}$ is the excitation energy of the level in question.

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3. J. M. Berger, Ap. J. 124, 550 (1956).

4. D. Schluter, Z. Astrophys. 61, 67 (1965) and private communication.

5. H. Griem, Plasma Spectroscopy, McGraw Hill Book Co., New York (1964).

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14407132 THURSDAY, MAY 11, 1967          NRL ALGOL VERSION OF  5/01/67
        BEGIN                                                                        SC  11  010
                                                            START OF SEGMENT **********    2
        COMMENT                                                                      SC  21  010
            THIS PROGRAM HAS BEEN WRITTEN TO CALCULATE THE SPECTRAL RADIANCE         SC  21  010
        OF AN ARC DISCHARGE AT ITS SURFACE( NORMAL ) DUE ONLY TO RADIANT             SC  21  010
        CONTRIBUTIONS FROM ALONG THE LINE OF SIGHT OF THE DIAMETER WHICH MAY         SC  21  010
        OR MAY NOT HAVE A SPATIAL TEMPERATURE GRADIENT , THIS PROGRAM                SC  21  010
        INITIATES BY FIRST READING FROM DISK FILES SPECTROSCOPIC DATA                SC  21  010
        INVOLVING BOUND-BOUND TRANSITIONS FOR THE PARTICULAR GAS IN  QUESTION        SC  21  010
        -- SUCH AS UNPERTURBED LINE FREQUENCIES AND THEIR CORRESPONDING              SC  21  010
        OSCILLATOR STRENGTHS, ELECTRON IMPACT SHIFTS AND WIDTHS,EXCITATION           SC  21  010
        ENERGIES,AND STATISTICAL WEIGHT PARAMETERS ,WITH THIS INFORMATION (          SC  21  010
        IN ADDITION TO THE ABOVE INPUT ,         THE PROGRAM READS IN  PARTICLE      SC  21  010
        NUMBER DENSITIES AND INTERNAL ATOMIC PARTITION FUNCTIONS       )             SC  21  010
        THE PROGRAM THEN TAKES THE INITIAL BAND PASS INPUT AND CALCULATES            SC  21  010
        WAVELENGTH INCREMENTS SUCH THAT ALL LINE PEAKS FOR ALL LINES THEREIN         SC  21  010
        FOR ALL TEMPERATURES ASSIGNED TO THE PROFILE ARE INCLUDED .                  SC  21  010
            FOR BOUND-BOUND TRANSITIONS INVOLVING GROUND STATE. A CALCULATION        SC  21  010
        OF RESONANCE LINE BROADENING IS ADDED TO THE ELECTRON IMPACT WIDTH--         SC  21  010
        ALL LINE PROFILES ARE ASSUMED TO BE OF THE LORENTZ TYPE .                    SC  21  010
            WITH THE ABOVE INFORMATION SPECTRAL ABSORPTIVITIES DUE TO THE            SC  21  010
        BOUND-BOUND- TRANSITIONS ARE  CALCULATED AND ADDED TO A BASE CONTINUUM       SC  21  010
        VALUE WHICH IS SPECIFIED BY INPUT , FOR XENON GAS THE CONTINUUM SPECTRAL     SC  21  010
        ABSORPTIVITIES ARE CALCULATED DIRECTLY USING  SCHLUTERS BOUND - FREE         SC  21  010
        ZETA TABLES CORRECTING A HYDROGENIC B-F EXPRESION WHICH IS THEN SUMMED       SC  21  010
        TO AN ADJUSTED HYDROGENIC FREE-FREE EXPRESSION---THE SUM  BEING ADDED TO     SC  21  010
        THE BOUND-BOUND VALUES.                                                      SC  21  010
            ONCE THE SPECTRAL ABSORPTIVITIES HAVE BEEN CALCULATED  THE               SC  21  010
        PROGRAM SOLVES THE RADIANT HEAT TRANSFER EQUATION ALONG THE ARC DIAMETER     SC  21  010
         , THE SPECRAL RADIANCE IS THEN PRINTED OUT AND PLOTTED  AS A FUNCTION       SC  21  010
        OF WAVELENGTH , IN ADDITION TO THIS OUTPUT THE PROGRAM WILL IF CALLED        SC  21  010
        UPON CALCULATE AND PLOT AS A FUNCTION OF WAVELENGTH THE SPECTRAL             SC  21  010
        RADIANT EMITTANCE (PRINTING OUT THE RADIANT EMITTANCE FOR THE BAND PASS)     SC  21  010
        AT  THE SURFACE  OF A  HOMOGENEOUS CYLINDRICAL ARC  FOR ANY OR  ALL          SC  21  010
        TEMPERATURES ASSIGNED TO THE PREVIOUS TEMPERATURE PROFILE FOR ANY NUMBER     SC  21  010
        OF DIFFERENT ARC DIAMETERS. FOR THE ABOVE TEMPERATURES THE PROGRAM WILL      SC  21  010
        PLOT THE SPECTRAL ABSORPTIVITIES AS A FUNCTION OF WAVELENGTH,                SC  21  010
            THIS PROGRAM HAS BEEN WRITTEN FOR THE FOLLOWING ATOMIC GASES--           SC  21  010
        SODIUM  (ATOMIC NUMBER= 11   )                                               SC  21  010
        POTASSIUM  (ATOMIC NUMBER =19   )                                            SC  21  010
        XENON  (ATOMIC NUMBER =54   )                          ;                     SC  21  010
        COMMENT                                                                      SC  21  010
        THIS PROGRAM CONTAINS TEN READ STATEMENTS FOR INPUT CARDS WHICH ARE          SC  21  010
        LISTED BELOW IN ORDER OF CALL AND VARIABLE CONCERNED----                     SC  21  010


        1 ) NMAX,NT,LAMMIN,LAMMAX,QMAX,LAM,NLAM,DRP,LY,LX,ATNUM,                     SC  21  010
        2 ) SCH[TEMPERATURE, WAVELENGTH(MICRONS)] ,                                  SC  21  010
        3 ) QD,ND,NE,DEL[TEMPERATURE] ,                                              SC  21  010
        4 ) T[M] ,                                                                   SC  21  010
        5 ) R[T] ,                                                                   SC  21  010
        6 ) PRESS ,                                                                  SC  21  010
        7 ) KONT ,                                                                   SC  21  010
        8 ) MARK ,                                                                   SC  21  010
        9 ) PLOTR[T] ,                                                               SC  21  010
        10) D[T] ,                                                                   SC  21  010
        ------------------------------------------------------------------------     SC  21  010
        THE ABOVE VARIABLES ARE DEFINED BELOW                                        SC  21  010
                                             - 1 -                                   SC  21  010
        NMAX   (INTEGER)  MAXIMUM NUMBER OF ATOMIC LEVELS LISTED ON DISK FILES       SC  21  010
                          READ1 AND READ2 .                                          SC  21  010
        NT    (INTEGER)   NUMBER OF TEMPERATURES ON DISK FILE READ3 FOR WHICH        SC  21  010
                          THE ELECTRON IMPACT SHIFTS AND WIDTHS HAVE BEEN            SC  21  010
                          CALCULATED .                                               SC  21  010
        LAMMIN (REAL)     MINIMUM WAVELENGTH(ANGSTROM UNITS ) OF THE                 SC  21  010
                          DESIRED BAND PASS                                          SC  21  010
        LAMMAX (REAL)     MAXIMUM WAVELENGTH(ANGSTROM UNITS ) OF THE                 SC  21  010
                          DESIRED BAND PASS                                          SC  21  010
        QMAX (INTEGER)    TOTAL NUMBER OF RADIAL TEMPERATURES  OF THE ARC            SC  21  010
                          TEMPERATURE PROFILE .                                      SC  21  010
        LAM   (REAL)      A MINIMUM INCREMENT OF THE WAVELENGTH BAND PASS  (         SC  21  010
                          ANGSTROM UNITS)---THIS VALUE CAN BE ZERO IF THE ATOMIC     SC  21  010
                          LINES ARE MORE THAN A FEW ANGSTROMS APART .                SC  21  010
        NLAM (INTEGER)    TOTAL NUMBER OF  INCREMENTS DESIRED IN THE  BAND           SC  21  010
                          PASS   (NOT TO EXCEED 1022 )   .                           SC  21  010
        DRP   (REAL)      AN INCREMENT OF BAND PASS (ANGSTROM UNITS) BEYOND          SC  21  010
                          INPUT  BAND PASS WHICH ALLOWS LINES IN THIS INCREMENT      SC  21  010
                          TO CONTRIBUTE TO THE INPUT BAND PASS SPECTRUM .            SC  21  010
        LY    (REAL)      LENGTH(INCHES) OF Y AXIS FOR PLOTS .                       SC  21  010
        LX    (REAL)      LENGTH(INCHES) OF X AXIS FOR PLOTS .                       SC  21  010
        ATNUM (REAL) ATOMIC NUMBER OF GAS ,                                          SC  21  010
                                             -2-                                     SC  21  010
        SCH    ( TWO DIMENTIONAL ARRAY)  SCHLUTERS ZETA FACTORS FOR XENON            SC  21  010
                          MUST BE INPUTED IN SPECIAL FORM,                           SC  21  010
                                             - 3 -                                   SC  21  010
        QD    (ARRAY)     ATOMIC INTERNAL PARTITION FUNCTION                         SC  21  010
        ND    (ARRAY)     NEUTRAL PARTICLE DENSITY (1/CM3 )   .                      SC  21  010
        NE    (ARRAY)     ELECTRON NUMBER DENSITY(1/CM3)   .                         SC  21  010
        DEL    (ARRAY)    IONIZATION POTENTIAL LOWERING VALUE (1/CM)      .          SC  21  010
                                             - 4 -                                   SC  21  010
        T     (ARRAY)      DESIRED TEMPERATURE PROFILE( DEG. KELVIN )                SC  21  010
```

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                    CORRESPONDING TO THE RADIAL VALUES BELOW ,                        SC   2:   010
                                    - 5 -                                             SC   2:   010
R     (ARRAY)       RADIAL VALUES (CM) CORRESPONDING TO THE ABOVE T                   SC   2:   010
                                    -6 -                                              SC   2:   010
PRESS (REAL)    PRESSURE OF ARC ( ATMOSPHERE  )  .                                    SC   2:   010
                                    - 7 -                                             SC   2:   010
KONT (REAL)         BASE VALUE FOR AN APPROXIMATE CONTINUUM ABSORPTIVITY              SC   2:   010
                     ( 1/CM)  .                                                       SC   2:   010
                                    - 8-                                              SC   2:   010
MAXN (INTEGER)      DESIRED NUMBER OF ABSORPTIVITY AND SPECTRAL EMITTANCE             SC   2:   010
                    CONSTANT TEMPERATURE PLOTS  .                                     SC   2:   010
                                    - 9 -                                             SC   2:   010
PLOTKT (ARRAY)      INDICES OF TEMPERATURES  TO BE USED FOR THE ABOVE                 SC   2:   010
                    PLOTS    .                                                        SC   2:   010
                    PLOTS ( THE FIRST TEMPERATURE LISTED IN " T " WOULD               SC   2:   010
                     BE 1 , THE SECOND TEMPERATURE IN " T " BEING  2 ECT,             SC   2:   010
                                    - 10 -                                            SC   2:   010
D     (REAL)        THE  THE ARC DIAMETER (CM) FOR THE SPECTRAL EMITTANCE             SC   2:   010
                    CALCULATION FOR THE FIRST TEMPERATURE INDEX LISTED IN             SC   2:   010
                    PLOTKT,UP TO MAXN  D VALUES CAN BE LISTED, EACH                   SC   2:   010
                    WILL BE FOR ONE  PLOTKT INDEX  (INPUT ON SEPARATE                 SC   2:   010
                    CARDS )   ;                                                       SC   2:   010
BEGIN                                                                                 SC   2:   010
FILE IN READF1 DISK SERIAL "LS" "READF1" (2,10,300);                                  SC   2:   010
                                                                START OF SEGMENT **********     3
FILE IN READF2 DISK SERIAL "LS" "READF2" (2,10,300);                                  SC   3:   3:2
FILE OUT PRINTER A(2,15) ;                                                            SC   3:   7:0
FILE IN READER (2,10) ;                                                               SC   3:  10:2
FILE IN READF3 DISK SERIAL "LS" "READF3" (2,10,300);                                  SC   3:  14:0
FORMAT F1(I3,I2,R12.3,R12.3,I2,R12.3,E18.6,E18.6),                                    SC   3:  17:2
                                                                START OF SEGMENT **********     4
        F2(E18.6) ,                                                                   SC   4:  17:2
        F3("2,I2,R12.3,E18.6,E18.6,R12.3)   ,                                         SC   4:  17:2
            F4(I2,R12.3,E18.6,E18.6) ,                                                SC   4:  17:2
            F5(A18,6(E15.3)),                                                         SC   4:  17:2
            F6(E18.6,6(E15.3));                                                       SC   4:  17:2
                                                                  4 IS   45 LONG, NEXT SEG     3
FORMAT FARRAY (/A10,6E15.6/(A10,6E15.6)) ;                                            SC   3:  17:2
                                                                START OF SEGMENT **********     5
                                                                  5 IS   12 LONG, NEXT SEG     3
REAL NLAM,LY,LX ;                                                                     SC   3:  17:2
REAL ARRAY SCH[0:15,0:81] ; INTEGER JJ,DD     ;                                       SC   3:  17:2
INTEGER ATNUM ;                                                                       SC   3:  19:2
REAL LAM, DRM ;                                                                       SC   3:  19:2
REAL LAMMAX, LAMMIN ;                                                                 SC   3:  19:2


REAL ARRAY  XLAM[0:30] ;                                                              SC   3:  19:2
     REAL A,B,C,F,G,H,  DD,X ; ARRAY SUM1[0:200] ; REAL NUMIN,N MAX ,NN;              SC   3:  21:1
     ARRAY EI,NU ,GFMN[0:200] ; INTEGER ARRAY NI,MI[0:200] ;                          SC   3:  23:0
     INTEGER Z,ZZ ;                                                                   SC   3:  27:1
     INTEGER ....AX ;                                                                 SC   3:  27:1
     INTEGER ZZZ ;                                                                    SC   3:  27:1
     INTEGER I,N,M,K,KSTIR,NMAX,      IMAX,IT,NT ,KMAX; ARRAY NU[0:1020];             SC   3:  27:1
ARRAY  AMP[0:1020] ;                                                                  SC   3:  24:0
REAL XIX ;                                                                            SC   3:  
COMMENT INTERPOLATION ROUTINE FOR SCHLUTERS ZETA FACTORS ;                            SC   3:  
REAL PROCEDURE SCHLUTER(A,H) ;                                                        SC   3:  30:3
     VALUE A,H ; REAL A,H ;                                                           SC   3:  30:3
          BEGIN                                                                       SC   3:  30:3
              REAL N,NMAX,NMIN,M,MMAX,MMIN,YU ,YL ;                                   SC   3:  30:3
                                                                START OF SEGMENT **********     6
              N:=H/M ; A:=A/2000 ;                                                    SC   6:   0:0
              NMIN:=ENTIER(N*R+10) ;                                                  SC   6:   2:2
              NMAX:=NMIN+1 ;                                                          SC   6:   5:1
              MMIN:=ENTIER(M*A+3) ;                                                   SC   6:   6:2
              MMAX:=MMIN+1 ;                                                          SC   6:   9:1
              YU:=SCH[MMAX,NMIN]x(NMAX-N)+SCH[MMAX,NMAX]x(N-NMIN) ;                   SC   6:  10:2
              YL:=SCH[MMIN,NMIN]x(NMAX-N)+SCH[MMIN,NMAX]x(N-NMIN) ;                   SC   6:  15:3
              SCHLUTER:=YLx(MMAX-M)+YUx(M-MMIN) ;                                     SC   6:  21:0
          END OF SCHLUTER PROCEDURE ;                                                 SC   6:  24:1
                                                                  6 IS   32 LONG, NEXT SEG     3
            $$ A CALC  P                                             00100000 SC   4:  31:3
COMMENT CALCUMP;                                                     00000000 SC   3:  31:3
COMMENT DS CAN  ,                                                    99999999 SC   4:  
READ(READER,/,NMAX,NT,LAMMIN,LAMMAX,AMAX,LAM,NLAM,DRM,LX,LY,ATNUM) ;                  SC   3:  
ZZZ:=NT ;                                                                             SC   4:  
IF ATNUM ... THEN                                                                     SC   4:  
READ(READER,/, FOR JJ:=1 STEP 1 UNTIL 5 DO FOR DD:=1 STEP 1 UNTIL 81 DO               SC   3:  
SCH[JJ,DD] ) ;                                                                        SC   3:  77:0
          BEGIN                                                                       SC   4:  
COMMENT DD TIME FOR READING  FROM DISK FILE SPECTROSCOPIC DATA ;                      SC   3:  
          REAL YY, LAMBDA ;                                                           SC   3:  
                                                                START OF SEGMENT **********    27
          REAL DS ;                                                                   SC  27:   0:0
      LABEL START,EXIT,START1,EXIT1,START2;                                           SC  27:   0:0
          REAL ARRAY T[0:QMAX] ;                                                      SC  27:   0:0
          ARRAY NE,TEMP,ND,DS,DEL       [0:NT] ;                                      SC  27:   2:3
          ARRAY KAPPA[0:QMAX] ;                                                       SC  27:   6:2
          ARRAY  ...D[0:NT,0:NMAX];                                                   SC  27:   9:1
              ARRAY JJ[0:NMAX]  ;                                                     SC  27:  13:2
          ARRAY J..[0:NMAX] ;                                                         SC  27:  14:1
```

```
        READ(READF1,/,A,B,C);                                              SC  271  1911
IF ATNUM=5A THEN                                                           SC  271  3113
        READ(READF1,/,FOR I+1          TIL NMAX DO (N,A,A,A,A,    J[I],    SC  271  3212
        E[I]));                                                            SC  271  4613
ELSE                                                                       SC  271  4811
        READ(READF1,/,FOR I+1 STEP 1 UNTIL NMAX DO (N,A,A,A,A,A,J[I],      SC  271  5313
        E[I]));                                                            SC  271  6910
                          REWIND (READF1); LOCK(READF1) ;                  SC  271  7513
FOR  I+1 STEP 1 UNTIL NMAX DO JJ[I]+J[I]  ;                                SC  271  7911
        READ(READF2,/,A,B,C,F,G);                                          SC  271  8313
        I+0 ;                                                              SC  271  9813
    LAMMIN+LAMMIN×B+B ;                                                    SC  271  9912
    LAMMAX+LAMMAX×B+A ;                                                    SC  271  10013
    NUMIN+1/LAMMAX ;                                                       SC  271  10210
NUMAX+1/LAMMIN ;                                                           SC  271  10311
OBP+OBP×B+B ;                                                              SC  271  10412
        C+.58723××NUMIN/(1+NUMIN×OBP) ; F+NUMAX×OBP ;                      SC  271  10513
        IF F≥1 THEN H+.58723××7 ELSE H+.58723××NUMAX/(1-F);                SC  271  10913
    START:                                                                 SC  271  11811
        READ(READF2,/,N,M,OS,YY,LAMBDA )[EXIT] ;                           SC  271  11910
        IF M≥N+1 THEN                                                      SC  271  13513
                        IF YY≥C THEN IF YY≤H THEN                          SC  271  13710
            BEGIN                                                          SC  271  13912
            REAL A ;                                                       SC  271  14010
                                                       START OF SEGMENT **********   28
            IF ATNUM=8) THEN IF N=    EN IF M=2 OR M=4 THEN OS+OS×.3 ;     SC  281   010
            I+I+1 ;                                                        SC  281   510
            A+YY/.58723× ;                                                 SC  281   711
            LAMBDA+1/A   ;                                                 SC  281   812
                        GFMN[I]+OS×A×(2×J[N]+1)/32921I.93 ;                SC  281   913
            NUO[I]+A ;                                                     SC  281  1313
            NI[I]+N ; I[I]+M ; EI[I]+E[N] ;                                SC  281  1510
    WRITE (PRINTER,F3,,    ,M    , LAMBDA,NUO[I],GFMN[I],EI[I]) ;          SC  281  1910
            END OF IF STATEMENT ;                                          SC  281  3811
                                                       28 IS    39 LONG, NEXT SEG   27
            GO TO START ;                                                  SC  271  14110
    EXIT : REWIND(READF2) ;  LOCK(READF2) ;                                SC  271  14112
     ZZ+IMAX+1 ;                                                           SC  271  14512
        READ(READF3,/,,,B,C,F,G);                                          SC  271  14613
    START1:                                                                SC  271  14113
        IT+0 ;                                                             SC  271  14210
    START2:                                                                SC  271  14213
        READ(READF3,/,,,B,C,F,G)[EXIT1]                                    SC  271  14310
        IF B=0 THEN GO TO START2 ;                                         SC  271  17813
        IF B=1 THEN                                                        SC  271  18010




            BEGIN                                                          SC  271  18013
            IT+IT+1 ; TEMP[IT]+C ; W[IT,N]+F ; U[IT,N]+G ;                 SC  271  18111
    WRITE(PRINTER,F4,N,C,F,G) ;                                            SC  271  18113
            END ;                                                          SC  271  20111
XIX+ EMP[1]/1000 ;                                                         SC  271  20111
        READ(READF3,/,,,B,C,F,G) ;                                         SC  271  20213
        IF IT<NT THEN GO TO START2 ELSE GO TO START1 ;                     SC  271  21713
    EXIT1 : REWIND(READF3) ;  LOCK(READF3) ;                               SC  271  21912
        READ(READER,/,FOR IT+1 STEP 1 UNTIL NT DO [UD[IT],ND[IT], NE[IT]   SC  271  22312
       ,DEL[IT] ]);                                                        SC  271  23313
        READ(READER,/,FOR G+1 STEP 1 UNTIL GMAX DO T[G] ]);                SC  271  24113
          BEGIN                                                            SC  271  25413
COMMENT DETERMINE  FREQUENCY  AND WAVELENGTH ARRAYS WHICH INCLUDE ALL      SC  271  25413
PEAK LINE VALUES FOR ALL TEMPERATURES LISTED  IN PROFILE  ;                SC  271  25413
        REAL NNU; REAL ARRAY SNU[0:1000] ;                                 SC  271  25413
                                                       START OF SEGMENT **********   29
        REAL H,AA ;INTEGER NI ;                                            SC  291   113
        LABEL EXIT2; REAL DELNU; INTEGER JMAX ,J ;                         SC  291   113
    REAL DELLAM ;                                                          SC  291   113
        REAL Q1,Q2,Q3 ;                                                    SC  291   113
        J+0 ;                                                              SC  291   113
        FOR G+1 STEP 1 UNTIL GMAX DO                                       SC  291   212
            BEGIN                                                          SC  291   410
            IT+ENTIER(.3×XIX×I×T[G]/1000) ;                                SC  291   410
            IF IT ≥NT  THEN IT+NT -1 ;                                     SC  291   410
            Q3+Q3-IT ,                                                     SC  291  1012
            H+ E[IT] ;                                                     SC  291  1113
            NN+H×((E[IT+1]/H)+Q3)××-1A ;                                   SC  291   213
            FOR I+1 STEP 1 UNTIL ZZ DO                                     SC  291  1713
                BEGIN H+NI[I]; N+NI[I];                                    SC  291  2110
                UU+[U[IT,M]-U[IT,N]]×(1-Q3)+(U[IT+1,M]-U[IT+1,N])×Q3 ;     SC  291  2310
                UD+NNN×UD ;                                                SC  291  3113
                A+NUO[I]+UD;                                               SC  291  3311
                IF A>  MIN THEN                                            SC  291  3413
                IF A<  MAX THEN                                            91  3512
                    BEGIN                                                  291  3A1
                    J+J+1 ;                                                SC  291  3712
                    SNU[J]+A ;                                             SC  291  3812
                    END ;                                                  C  291  3913
                END OF I LOOP ;                                            SC  291  3913
            END OF G  LOOP ;                                               SC  291  4210
            JMAX+J ;                                                       SC  291  4411
NU[1]+1/(LAMB[1]+LAMMIN ) ;                                                SC  291  4510
        DELLAM+(LAMMAA-LAMMIN)/NLAM ;                                      SC  291  4713
        FOR K+1 STEP 1 WHILE LAMB[K]<LAMMAX DO                             SC  291  4912
```

```
            BEGIN                                                                  SC  291  5A10
            IF K≥TU20 THEN GO TO EXIT2 ;                                           SC  291  5A10
            H←LAMB[K] ;                                                            SC  291  5511
            A←H÷DELLAM ;                                                           SC  291  5A11
            H←H←LAM×B←4 ;                                                          SC  291  5712
            A←A←LAM×B←5 ;                                                          SC  291  5911
            FOR J←1 STEP 1 UNTIL JMAX DO                                           SC  291  A110
                BEGIN                                                              SC  291  A310
                C←1/SNU[J] ;                                                       SC  291  A510
                IF C>B THEN IF C<A THEN A←C                      ;                 SC  291  AA12
                END ;                                                              SC  291  A713
            LAMB[K+1]←A ;                                                          SC  291  7010
            NU[K+1]←1/A ;                                                          SC  291  7113
         END OF K LOOP ;                                                           SC  291  7A10
EXIT2:  KMAX←K−1 ;NUMAX←NU[K−1] ;  Z←KMAX ;                                        SC  291  7A12
LAMMAX←LAMB[K−1] ;                                                                 SC  291  7812
END OF FREQUENCY AND WAVELENGTH ARRAYS ;                                           SC  291  4010
                                                        29 IS    83 LONG, NEXT SEG    27
BEGIN COMMENT RADIANT INTENSITY CALCULATION AT SURFACE OF CYLINDRICAL              SC  271 25A10
               ARC COLUMN FROM ALONG LINE OF SIGHT OF DIAMETER HAVING              SC  271 25A12
              SPATIAL TEMPERATURE GRADIENT ;                                       SC  271 25A10
         REAL AA, BB,CC,LL,    XX,GG,FF       ;                                    SC  271 25A10
                                                     START OF SEGMENT **********      30
REAL KK ;                                                                          SC  301   010
INTEGER ARRAY PLOTKT[0:QMAX] ;                                                     SC  301   010
ARRAY KT[0:QMAX,0:Z−1] ;                                                           SC  301   213
ARRAY KP,LK,PNU0,BEXP,MAXNU,MINNU[0:QMAX,0:ZZ] ;                                   SC  301   711
INTEGER MAXN ;                                                                     SC  301  1212
BOOLEAN PLOTTEST ;                                                                 SC  301  1212
REAL C1,C2,INTERP,A,B,C ,C3 ,   G ;                                                SC  301  1212
REAL H;                                                                            SC  301  1212
REAL YMIN,DY,XMIN,DX;                                                              SC  301  1212
INTEGER I,J,K,IMAX,JMAX,KMAX,N,NMAX ;                                              SC  301  1212
NMAX←Z−1 ;                                                                         SC  301  1212
JMAX←QMAX−1 ;                                                                      SC  301  1313
IMAX←2×JMAX ;                                                                      SC  301  1510
KMAX←A×JMAX ;                                                                      SC  301  1611
BEGIN                                                                              SC  301  1712
REAL ARRAY    FINU[0:NMAX]  ;                                                      SC  301  1712
                                                     START OF SEGMENT **********      31
REAL ARRAY LLAMB[0:1020]   ;                                                       SC  311   213
REAL UN ;                                                                          SC  311   A12
REAL PRESS ;                                                                       SC  311   A12
REAL ARRAY   R       [0:JMAX] ;                                                    SC  311   A12
REAL ARRAY NT,NR,KKAPPA,IB[0:IMAX] ;                                               SC  311   711


REAL ARRAY DELTAU,TAU,XIB,DELINU  ,INU[0:KMAX] ;                                   SC  311  1013
LABEL STARTA,EXITA ;                                                               SC  311  1A12
LABEL STARTS;                                                                      SC  311  1A12
REAL Q3,H ; INTEGER IT ;                                                           SC  311  1A12
         REAL W ;                                                                  SC  311  1412
REAL T4,TT4,ZETA    ;                                                              SC  311  1412
REAL KUNT,Q8,Q9 ;                                                                  SC  311  1A12
READ (HEADER,/,FOR J←0 STEP 1 UNTIL JMAX DO R[J] )[EXITA];                         SC  311  1A12
FOR J←0 STEP 1 UNTIL JMAX DO T[J]←T[J+1] ;                                         SC  311  2813
WRITE (PRINTER,FARRAY,"      T",FOR J←0 STEP 1 UNTIL JMAX DO T[J]);                SC  311  3A11
WRITE (PRINTER,FARRAY,"      R",FOR J←0 STEP 1 UNTIL JMAX DO R[J]);                SC  311  5111
FOR J←0 STEP 1 UNTIL JMAX DO                                                       SC  311  5811
    BEGIN COMMENT GENERATE NEW TEMP AND RADIUS TABLES ;                            SC  311  6910
    NT[2×J]←T[J] ;                                                                 SC  311  6910
    NR[2×J]←R[J] ;                                                                 SC  311  7110
    IF (2×J+1)<IMAX THEN                                                           SC  311  7310
        BEGIN                                                                      SC  311  7A13
        A←R[J+1] ;                                                                 SC  311  7511
        B←R[J] ;                                                                   SC  311  7A13
        C←A+B ;                                                                    SC  311  7713
        INTERP←(.25×A+.75×B)/C ;                                                   SC  311  7010
        NT[2×J+1]←T[J]+(T[J+1]−T[J])×INTERP ;                                      SC  311  8113
        NR[2×J+1]←.5×C ;                                                           SC  311  8A13
        END ;                                                                      SC  311  9012
    END OF GENERATING NEW TEMPERATURE AND RADIUS TABLES ;                          SC  311  9012
WRITE (PRINTER,FARRAY,"      NR",FOR I←0 STEP 1 UNTIL IMAX DO NR[I]);              SC  311  9113
WRITE (PRINTER,FARRAY,"      NT",FOR I←0 STEP 1 UNTIL IMAX DO NT[I]);              SC  311 11111
C1← 1.47429@−24   ;                                                                SC  311 12811
C2← 4.79932@−11   ;                                                                SC  311 12910
PLOTTEST←FALSE ;                                                                   SC  311 12913
READ(HEADER,/,PRESS) ;                                                             SC  311 13012
WRITE(PRINTER,FARRAY,"PRESS=",PRESS) ;                                             SC  311 14013
READ(HEADER,/,KUNT) ;                                                              SC  311 15A11
READ(HEADER,/,MAXN)[STARTA] ;                                                      SC  311 16113
READ (HEADER,/, FOR I←1 STEP 1 UNTIL MAXN DO PLOTKT[I])[STARTA] ;                  SC  311 17013
PLOTTEST←TRUE ;                                                                    SC  311 18A13
STARTA:                                                                            SC  311 1A512
       BEGIN COMMENT DETERMINE KAPPA ARRAY FOR A GIVEN FREQUENCY THEN              SC  311 18A10
       TAKE THIS ARRAY AND CALCULATE THE ARC RADIANT TRANSFER ;                    SC  311 18A10
       REAL Q1,Q2,Q3 ;                                                             SC  311 19610
                                                     START OF SEGMENT **********      32
REAL ARRAY Q11[0:100]     ;                                                        SC  321   010
         REAL Q4,Q5,Q6 ;                                                           SC  321   113
              LABEL A10,CONTINUE ;                                                 SC  321   113
           LABEL A5A  ;                                                            SC  321   113
```

APPENDIX D

WHITTAKER AND GAMMA FUNCTIONS - DESCRIPTION OF TWO ALGOL PROCEDURES

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ABSTRACT

This report describes the development and testing of two computer algorithms WOG and GAMMAC required in connection with computation of spectral properties of plasma arcs being carried out for Dr. C. H. Church of Quantum Electronics R & D. The algorithm WOG computes the irregular Whittaker function $W_{\eta,\ell+1/2}$ for real positive non-integral η, and for ℓ a non-negative integer. GAMMAC computes the function $\Gamma(z)$ for z real or complex. A very good accuracy has been obtained from both of these algorithms. GAMMAC is used in WOG, which calculates one of the four confluent hypergeometric functions needed in the calculation of transitions between eigenstates described by the Coulomb wave functions.

```
            SCHLUTER(TT,,584)*(EXP(584/C)-1)/(EXP(BB/C)-1) ELSE          SC  321 23312
            SCHLUTER(TT,,BB)  ;                                           SC  321 23912
     KONT ←(4.04@-7*HHKT[Q]/(BB+3)*EXP(-(07834.4-GG)/C)*                  SC  321 24110
           ( .A + EXP(1#3/C) + ZETA*(EXP(BB/C)-1) ) +B*                   SC  321 24611
           ( IF BB≥ 2.935@5/3 THEN 9@-17 + (2.59*2.93)*@-17-             SC  321 25110
           7.77*BB*@-22  ELSE 0 ) )*Q7     ;                              SC  321 25812
END OF KONT    ;                                                          SC  321 25811
IF Q9>.001*KONT THEN BEGIN                                                SC  321 25811
Q9←SQRT(1000*Q8/KONT-1) ;                                                 SC  321 26010
MAXNU[Q,I]←B3+AA*Q9 ;                                                     SC  321 26213
MINNU[Q,I]←B3-AA*Q9 ;                                                     SC  321 26513
END ELSE BEGIN                                                            SC  321 26813
MAXNU[Q,I]←0 ;                                                            SC  321 28710
 MINNU[Q,I]←@20 ;                                                         SC  321 28910
END ;                                                                     SC  321 29110
END OF I LOOP ;                                                           SC  321 29110
END OF Q LOOP ;                                                           SC  321 29311
END ;                                                                     SC  321 29510
                                                         32 IS  298 LONG, NEXT SEG   31
N←0 ;                                                                     SC  311 18710
START5:                                                                   SC  311 18713
FF←NU[N+1] ;                                                              SC  311 18810
FOR Q←0 STEP 1 UNTIL QMAX-1 DO                                            SC  311 18912
BEGIN                                                                     SC  311 19410
             IT←ENTIER(Q3*X1X+1-T[Q]/1000) ;                              SC  311 19410
             IF IT ≥ZZZ THEN IT←ZZZ-1 ;                                   SC  311 19810
             Q3←Q3-IT ;                                                   SC  311 20012
             H←ND[IT]/UD[IT] ;                                            SC  311 20113
             H←H*(IND[IT+1]/UD[IT+1]/H)↑Q3) ;                             SC  311 20312
             H←DEL[IT] ;                                                  SC  311 20911
             GG←H*((DEL[IT+1]/H)↑Q3) ;                                    SC  311 21011
C←.6925*1  ] ;                                                            SC  311 21413
Q8←1-EXP(-FF/C) ;                                                         SC  311 21611
KK←0 ;                                                                    SC  311 21813
FOR I←1 STEP 1 UNTIL ZZ DO                                                SC  311 21912
IF FF≥MINNU[Q,I] THEN                                                     SC  311 22310
IF FF≤MAXNU[Q,I] THEN                                                     SC  311 22813
BEGIN                                                                     SC  311 22710
BB←BNUO[Q,I] ;                                                            SC  311 22712
LL←1/I((FF-BB)/LW[Q,I])↑2+1) ;                                            SC  311 22911
KK   ←KK       +Q8/BEXP[G,I]*KP[G,I]*LL ;                                 SC  311 23312
END OF I LOOP ;                                                           SC  311 23811
IF ATNUM=5A THEN                                                          SC  311 24012
BEGIN                                                                     SC  311 24111
Q7←Q8 ;                                                                   SC  311 24113

     BB←FF ;                                                              SC  311 24212
     TT←  IF TQ←T[Q]≤8000 THEN 8000 ELSE IF TQ≥16000 THEN 14000 ELSE TQ ; SC  311 24311
     ZETA ← IF BB≤1@A THEN 1.1 ELSE IF BB> 584 THEN                       SC  311 24810
            SCHLUTER(TT,,584)*(EXP(584/C)-1)/(EXP(BB/C)-1) ELSE           SC  311 25112
            SCHLUTER(TT,,BB)  ;                                           SC  311 25712
     KONT ←(4.04@-7*HHKT[Q]/(BB+3)*EXP(-(07834.4-GG)/C)*                  SC  311 25910
           ( .A + EXP(1#3/C) + ZETA*(EXP(BB/C)-1) ) +B*                   SC  311 26411
           ( IF BB≥ 2.935@5/3 THEN 9@-17 + (2.59*2.93)*@-17-             SC  311 26910
           7.77*BB*@-22  ELSE 0 ) )*Q7     ;                              SC  311 27212
END OF KONT    ;                                                          SC  311 27611
KAPPA[Q]←KK      +KONT ;                                                  SC  311 27511
END OF Q LOOP ;                                                           SC  311 27810
IF PLOTTEST       THEN FOR I←1 STEP 1 UNTIL MAXN DO                       SC  311 29510
BEGIN                                                                     SC  311 29710
Q←PLOTKT[I]-1 ;                                                           SC  311 29710
KT[Q,N]←KAPPA[Q] ;                                                        SC  311 29812
END ;                                                                     SC  311 30013
FOR J←0 STEP 1 UNTIL JMAX DO                                              SC  311 30310
     BEGIN COMMENT GENERATE NEW KAPPA TABLE ;                             SC  311 30410
     NKAPPA[2*J]←KAPPA[J] ;                                               SC  311 30410
     IF (2*J+1)<IMAX THEN                                                 SC  311 30610
          BEGIN                                                           SC  311 30713
          INTERP←(.25*P[J+1]+.75*P(J])/(R[J+1]+R[J])  ;                   SC  311 30811
          NKAPPA[2*J+1]←KAPPA[J]+(KAPPA[J+1]-KAPPA[J])*INTERP ;           SC  311 31312
          END ;                                                           SC  311 31812
     END OF CALCULATING NEW KAPPA TABLE ;                                 SC  311 31812
TAU[0]←0.0;                                                               SC  311 32013
FOR I←1 STEP 1 UNTIL IMAX DO                                              SC  311 32210
     BEGIN COMMENT CALCULATION OF OPTICAL DEPTH  ;                        SC  311 32510
     A←NR[I]   ;                                                          SC  311 32510
B←NR[I-1]   ;                                                             SC  311 32610
DELTAU[I]←NKAPPA[I-1]*(A-B)+(NKAPPA[I]-NKAPPA(I-1])*                      SC  311 32712
(A+3/3-(A-2*H/3)*H+2)/((A-B)*(A+B))   ;                                   SC  311 33113
     TAU[I]←TAU[I-1]+DELTAU[I] ;                                          SC  311 33912
     END OF CALCULATING OPTICAL DEPTH ;                                   SC  311 34211
[illegible]N←NU[N]←NU[N+1]*2.99793@10 ;                                   SC  311 34412
LLAMB[N]←A←LAMB[N+1]   ;                                                  SC  311 34712
LAMB[N]←A*B*B*(1-B-A*(6*.328+20A6B,1/(1#A-B-B/(A+2))+255,A/(41-B-B/(A+2)  SC  311 35010
))) ;                                                                     SC  311 35513
FOR J←0 STEP 1 UNTIL JMAX DO                                              SC  311 35811
     BEGIN COMMENT CALCULATE BLACK BODY ;                                 SC  311 36610
     C3←(NU[N]↑3)*1@-30 ;                                                 SC  311 36610
     IB[2*J]←          C3*C1/(EXP(C2*NU[N]/T[J])-1) ;                     SC  311 36812
     IF (2*J+1)<IMAX THEN                                                 SC  311 37313
          BEGIN                                                           SC  311 37512
```

```
        IH[2*J+1]←      C3←C1/(EXP(C2*NU[N]/NT[2*J+1]))−1) ;           SC  311: 37610
        END ;                                                           SC  311: 38213
    END ;                                                               SC  311: 38213
TAU[0]←0 ;                                                              SC  311: 38510
INU[0]←0 ;                                                              SC  311: 38611
FOR I←1 STEP 1 UNTIL IMAX DO                                            SC  311: 38712
    BEGIN                                                               SC  311: 39010
COMMENT CALCULATION OF SPECTRAL RADIANCE AT COLUMN SURFACE ;            SC  311: 39010
REAL ETM,A,B,C,D,F,A1,A2,A3,A4,B1,B2,B3,B4,B5 ;                         SC  311: 39010
                                                     START OF SEGMENT ..........  33
REAL BA ;                                                               SC  331:   010
ETM←EXP(BA×−TAU[IMAX]) ;                                                SC  331:   010
A←TAU[I−1] ;                                                            SC  331:   211
B←TAU[I] ;                                                              SC  331:   313
C←IH[I−1] ;                                                             SC  331:   413
F←IH[I] ;                                                               SC  331:   611
D←DELTAU[I] ;                                                           SC  331:   711
IF BS.01 THEN                                                           SC  331:   811
DELINU[I]←2×ETM×D×(A×C+F×B)/(A+B)                                       SC  331:   910
ELSE IF DS.01 THEN BEGIN                                                SC  331:  1312
A1←EXP(A×BA) ;A2←EXP(−A×BA) ;                                           SC  331:  1811
B1←(A1+A2) ;                                                            SC  331:  2210
B2←(A1−A2) ;                                                            SC  331:  2311
DELINU[I]←  D×(F×B1−(F−C)×B2 (A+B)) ;                                   SC  331:  2412
END  ELSE BEGIN                                                         SC  331:  2911
A1←EXP(A×BA) ; A2←EXP(−A×BA) ;                                          SC  331:  3110
A3←EXP(B×BA) ; A4←EXP(−B×BA) ;                                          SC  331:  3413
B1←A1+A2 ;B2←A1−A2 ;                                                    SC  331:  3512
B3←A3+A4 ;B4←A3−A4 ;                                                    SC  331:  4110
B5←(F−C)/D/(A+B) ;                                                      SC  331:  4312
DELINU[I]←    (F×B4−C×B2−2×B5×(B×B3−A×B1−B4+B2)) ;                      SC  331:  4611
END;                                                                    SC  331:  5310
INU[I]←INU[I−1]+DELINU[I] ;                                             SC  331:  5310
    END OF CALCULATING SPECTRAL RADIANCE  ;                             SC  331:  5513
                                                     33 IS   57 LONG, NEXT SEG  31
FINU[N]←INU[IMAX]×(LN*2)×8−10/2.99793 ;                                 SC  311: 39311
IF N=NMAX   THEN GO TO EXIT4 ;                                          SC  311: 39413
N←N+1 ;                                                                 SC  311: 39810
GO TO START5 ;                                                          SC  311: 39911
EXIT4:                                                                  SC  311: 40210
WRITE(PRINTER,FARRAY,"LAMBDA", FOR N←0 STEP 1 UNTIL NMAX DO LAMB[N]) ;  SC  311: 40210
WRITE (PRINTER,FARRAY,"    NU",FOR N←0 STEP 1 UNTIL NMAX DO NU[N]) ;    SC  311: 41811
WRITE (PRINTER,FARRAY,"   INU",FOR N←0 STEP 1 UNTIL NMAX DO FINU[N]);   SC  311: 43511
    BEGIN                                                               SC  311: 45211
COMMENT PLOT ROUTINE FOR SPECTRAL RADIANCE  ;                           SC  311: 45211


    BOOLEAN TRY  ;
                                                                        SC  311: 45211
                                                     START OF SEGMENT ..........  34
ALPHA ARRAY PALF[0:3] ;                                                 SC  341:   010
    ALPHA ARRAY YALF[0:7],XALF[0:3],BCD1[0:9],BCD2[0:8],BCD3[0:3] ;     SC  341:   113
    ALPHA ARRAY LALF[0:3] ;                                             SC  341:  1012
    FILL YALF[*] WITH                                                   SC  341:  1211
"   SPE","CTRAL ",                                                      SC  341:  1213
                                                     START OF SEGMENT ..........  35
                     " RADIA","NCE ( ","WATTS/","CM*2/S","TER/CM",      SC  341:  1410
" )    " ;                                                              SC  341:  1410
                                                     35 IS    5 LONG, NEXT SEG  34
    FILL XALF[*] WITH "WAVELE","NGTH (","ANGSTR","OMS)  " ;             SC  341:  1410
                                                     START OF SEGMENT ..........  36
                                                     36 IS    4 LONG, NEXT SEG  34
FILL PALF[*] WITH "PRESSU","RE =  ","     A","TM    " ;                 SC  341:  1513
                                                     START OF SEGMENT ..........  37
                                                     37 IS    4 LONG, NEXT SEG  34
    BCD1[0]←"SPECTR" ; BCD1[1]←"AL  RA" ; BCD1[2]←"DIANCE" ;            SC  341:  1712
    BCD1[3]←" AT SU" ; BCD1[4]←"RFACE " ; BCD1[5]←"OF CYL" ;            SC  341:  2111
    BCD1[6]←"INDRIC" ; BCD1[7]←"AL ARC" ; BCD1[8]←" COLUM" ;            SC  341:  2510
    BCD1[9]←"N     " ;                                                  SC  341:  2813
    BCD2[0]←"FROM A" ; BCD2[1]←"LONG L" ; BCD2[2]←"INE OF" ;            SC  341:  3010
    BCD2[3]←" SIGHT" ; BCD2[4]←" OF DI" ; BCD2[5]←"AMETER" ;            SC  341:  3313
    BCD2[6]←" HAVIN" ; BCD2[7]←"   A SP" ; BCD2[8]←"ATIAL " ;           SC  341:  3712
    BCD3[0]←"TEMPER" ; BCD3[1]←"ATURE " ; BCD3[2]←"GRADIE" ;            SC  341:  4111
    BCD3[3]←"NT .  " ;                                                  SC  341:  4510
PLOT(0.0,0.0,1019) ;                                                    SC  341:  4611
PLOT(0.0,0.1,−3) ;                                                      SC  341:  4712
    RSCALE(FINU,NMAX+1,1,LY,YMIN,DY);                                   SC  341:  4910
    AXIS(−.25 ,0,YALF,48,LY,90,YMIN,DY);                                SC  341:  5210
    RSCALE(LAMB,NMAX+1,1,LX,XMIN,DX) ;                                  SC  341:  5511
    AXIS(0,0,XALF,24,LX,0,XMIN,DX);                                     SC  341:  5811
    SYMBOL(1,LY+.5,.14,BCD1,0,60);                                      SC  341:  6111
    SYMBOL(1,LY+.29,.14,BCD2,0,54);                                     SC  341:  6411
    SYMBOL(1,LY+.09,.14,BCD3,0,24);                                     SC  341:  6711
    SYMBOL(1,LY−.11,.14,PALF,0,24) ;                                    SC  341:  7011
    NUMBER(1.72,LY−.11,.14,PRESS,0,3) ;                                 SC  341:  7311
    TRY←TRUE ;                                                          SC  341:  7513
    LINE(LAMB,FINU,NMAX+1,TRY) ;                                        SC  341:  7612
PLOT(LX+3,0,−3) ;                                                       SC  341:  7912
    END OF SPECTRAL RADIANCE PLOT ROUTINE  ;                            SC  341:  8112
                                                     34 IS  110 LONG, NEXT SEG  31
BEGIN                                                                   SC  311: 45310
COMMENT SPECTRAL EMITTANCE CALCULATIONS AND PLOT ROUTINE  ;             SC  311: 45310
COMMENT SIMPSON PROCEDURE ;                                             SC  311: 45310
```

```
REAL                                                                         SC 31: 45310
                                                          START OF SEGMENT **********   38
PROCEDURE SIMPSON(A,B,X,Y,N);                                                SC 38: 010
COMMENT N MUST BE EVEN;                                                      SC 38: 010
VALUE A,B,N;                                                                 SC 38: 010
REAL A,B,N,X,Y;                                                              SC 38: 010
BEGIN                                                                        SC 38: 010
REAL DX,DX2,SUM2,SUM4,BB,SUM;                                                SC 39: 010
                                                          START OF SEGMENT **********   39
IF N MOD 2 = 0 THEN BEGIN                                                    SC 39: 010
SUM2←SUM4←SUM←0;                                                             SC 39: 113
DX←(B-A)/(N);                                                                SC 39: 312
DX2←DX+DX; BB←B-DX+DX/4;                                                     SC 39: 511
FOR X←A+DX2 STEP DX2 UNTIL BB DO                                             SC 39: 813
SUM2←SUM2+Y;                                                                 SC 39: 1413
FOR X←A+DX STEP DX2 UNTIL BB DO                                              SC 39: 1612
SUM4←SUM4+Y;                                                                 SC 39: 2212
FOR X←A,B DO                                                                 SC 39: 2411
SUM←SUM+Y;                                                                   SC 39: 2911
SIMPSON←(SUM+2×SUM2+4×SUM4)×DX/3;                                            SC 39: 3110
END ELSE                                                                     SC 39: 3413
WRITE(PRINTER,<X5," N IS NOT AN INTEGER    ">) ;                             SC 39: 3413
                                                       40 IS     8 LONG, NEXT SEG   39
END OF PROCEDURE SIMPSON;                                                    SC 39: 3811
                                                       39 IS    42 LONG, NEXT SEG   38
REAL VDIV,DV,V,D,TAU,UDIV,A,U,U2,FF ;                                        SC 38: 010
INTEGER I; BOOLEAN TRY ; LABEL EXIT6 ;                                       SC 38: 010
SAVE ARRAY SINV[0:6] ;                                                       SC 38: 010
ALPHA ARRAY YALF[0:4],XALF[0:3],BCD1[0:4] ,BCD2[0:7] ;                       SC 38: 113
ALPHA ARRAY BCD3,BCD4[0:3]  ;                                                SC 38: 813
FILL YALF[*] WITH "SPECTR","AL RAD","IANT E","MITTAN","CE (WA",              SC 38: 1013
                                                          START OF SEGMENT **********   41
                     "TTS/CM","2/CM)" ;                                      SC 39: 1212
                                                       41 IS     7 LONG, NEXT SEG   38
FILL XALF[*] WITH "WAVELE","NGTH (", "ANGSTR","OMS ; " ;                     SC 39: 1212
                                                          START OF SEGMENT **********   42
                                                       42 IS     4 LONG, NEXT SEG   38
FILL BCD1[*] WITH "TEMPER","ATURE ","=       ", "    OF", "G, K   " ;        SC 38: 1411
                                                          START OF SEGMENT **********   43
                                                       43 IS     5 LONG, NEXT SEG   38
FILL BCD2[*] WITH                                                            SC 38: 1610
"RADIAN","T EMIT","TANCE ","=       ","  =  ","  (WAT","TS/CM","2)    ";    SC 38: 1612
                                                          START OF SEGMENT **********   44
FILL BCD3[*] WITH "ARC  D","IAMETE","R =   ","     CM"  ;                    SC 38: 1713
                                                       44 IS     8 LONG, NEXT SEG   38

                                                          START OF SEGMENT **********   45
                                                       45 IS     4 LONG, NEXT SEG   38
FILL BCD4[*] WITH "PRESSU","RE =  ","      ATM","    " ;                     SC 38: 1912
                                                          START OF SEGMENT **********   46
                                                       46 IS     4 LONG, NEXT SEG   38
VDIV←4;                                                                      SC 38: 2111
DV←1.57079633265/VDIV ;  V← -DV×.999999 ;                                    SC 38: 2210
FOR I←0 STEP 1 UNTIL VDIV DO                                                 SC 38: 2413
SINV[I]←SIN(V←V+DV)*2 ;                                                      SC 38: 2810
TRY← TRUE ;                                                                  SC 34: 3312
IF PLOTTEST THEN FOR I←1 STEP 1 UNTIL MAXN DO                                SC 38: 3411
BEGIN                                                                        SC 38: 3610
READ(READER,/,U)[EXIT6] ;                                                    SC 38: 3610
Q←PLOT<T[I]>1  ;                                                             SC 38: 4413
FOR N←0 STEP 1 UNTIL NMAX DO                                                 SC 38: 4411
    BEGIN                                                                    SC 38: 4710
    TAU← AT[Q,N]×U  ;                                                        SC 38: 4710
    UDIV←ENTIER(TAU×1.5) ;                                                   SC 38: 4911
    IF UDIV MOD 2≠0 THEN UDIV←UDIV+1 ;                                       SC 38: 5112
    IF UDIV<2 THEN UDIV←2  ;                                                 SC 38: 5412
    FF←NU[N] ;                                                               SC 38: 5612
    C3←(FF*3)×10*30;                                                         SC 38: 5712
    FINU[N]←C3×C1/(EXP(C2×FF/T[Q])-1)×(3.14159265358×4×                      SC 38: 5913
        4×( IF UDIV >100 THEN 0 ELSE                                         SC 38: 6411
            SIMPSON(0,1,U,SIMPSON(0,VDIV, V,EXP(-TAU×U/((U2×U*2)+            SC 38: 6611
                (1-U2)×SINV[V]))),VDIV)×U/(VDIV)×1.5707963268/VDIV))         SC 38: 7412
                ×(FF*2)×A*1)/2.99793 ;                                       SC 38: 8511
    END ;                                                                    SC 38: 8910
A←0 ;                                                                        SC 38: 9111
FOR N←1 STEP 1 UNTIL NMAX-1 DO                                               SC 38: 9210
A←A+(FINU[N]+FINU[N+1])×(LLAMB[N+1]-LLAMB[N])/2                              SC 38: 9612
WRITE(PRINTER,/,ARRAY,"LAMBDA",FOR N←0 STEP 1 UNTIL NMAX DO LLAMB[N]);       SC 38: 10410
WRITE(PRINTER,FARRAY,"   FNU",FOR N←0 STEP 1 UNTIL NMAX DO FINU[N]);         SC 38: 12211
WRITE(PRINTER,<X5,"FLUX DUE TO THIS BAND PASS",E18.4>,A) ;                   SC 38: 13911
                                                       47 IS    10 LONG, NEXT SEG   38
R← ENTIER(.43429×LN(A))       ;                                              SC 38: 14711
A←A/(10*R)   ;                                                               SC 38: 15010
AXIS(0,0,XALF,24,LX,0,XMIN,DX);                                              SC 38: 15311
ASCALE(FINU,NMAX+1,1,LY,YMIN,DY) ;                                           SC 39: 15611
AXIS(-.25,0,YALF,42,LY,90,YMIN,DY ) ;                                        SC 39: 15911
SYMBOL(1,LY+.5,.14,BCD1,0,30) ;                                              SC 38: 16212
NUMBER(2.68,LY+.5,.14,T[Q],0,0 ) ;                                           SC 38: 16512
SYMBOL(1,LY+.3,.14,BCD2,0,48) ;                                              SC 38: 16811
NUMBER(2.80 ,LY+.3,.14,A,0,4) ;                                              SC 38: 17111
NUMBER(4.00,LY+.3,.14,R,0,0) ;                                               SC 38: 17313
```

```
SYMBOL(I,LY+.I,.1A,BCO3,0,24) ;
NUMBER(2.44,LY+.I,.14,J,0,2) ;
SYMBOL(I,LY-.1,.IA,BCO4,0,24) ;                            SC  38: 17611
NUMBER(1.72,LY-.1,.IA,PRESS,0,3) ;                         SC  38: 17911
LINE(LAMB,FINU,NMAX,I,TRY) ;                               SC  38: 18113
PLOT(LX+3,0,-3 ) ;                                         SC  38: 18413
END OF I LOOP PLOTS ;                                      SC  38: 18711
EXIT6:                                                     SC  38: 19011
END OF SPECTRAL EMITTANCE CALCULATIONS AND PLOT ROUTINE ;  SC  38: 19211
                                                           SC  38: 19412
IF PLOTTEST THEN                                           SC  38: 19510
BEGIN                                        38 IS  209 LONG, NEXT SEG  31
COMMENT ABSORPTIVITY PLOT ROUTINE ;                        SC  31: 45410
BOOLEAN TRY;                                               SC  31: 45411
                                                           SC  31: 45413
ALPHA ARRAY YALF[0:4],XALF[0:3],BCOI[0:4] ;                SC  31: 45413
FILL YALF[*] WITH                            START OF SEGMENT ..........  48
"   SPE","CTRAL ",                                         SC  48:   010
                                                           SC  48:   511
                "ABSORP","TIVITY","(1/CM)" ;               SC  48:   513
                                             START OF SEGMENT ..........  49
    FILL XALF[*] WITH "WAVELE","NGTH (","ANGSTR","UMS)  " ; SC  48:  710
                                             49 IS    5 LONG, NEXT SEG  48
                                                           SC  48:   710
FILL BCOI[*] WITH "TEMPER","ATURE ","      ","    UE","G, K  " ;
                                             START OF SEGMENT ..........  50
                                             50 IS    4 LONG, NEXT SEG  48
                                                           SC  48:   513
TRY←TRUE ;                                   START OF SEGMENT ..........  51
FOR I←1 STEP 1 UNTIL MAXN DO                 51 IS    5 LONG, NEXT SEG  46
BEGIN                                                      SC  48:  1012
AXIS(0,0,XALF,24,LX,0,XMIN,DX);                            SC  48:  1111
Q←PLOTXT[I]-1 ;                                            SC  48:  1210
FOR N←0 STEP 1 UNTIL NMAX  DO                              SC  48:  1210
FINU[N]←KT[Q,N] ;                                          SC  48:  1510
RSCALE(FINU,NMAX,I,1,LY,   YMIN,DY) ;                      SC  48:  1612
    AXIS(-.25 ,0,YALF,30,LY,90,YMIN,DY);                   SC  48:  1810
SYMBOL(I,LY+.5,.IA,BCOI,0,30);                             SC  48:  2212
NUMBER(2.68,LY+.5,.14,T[Q],0,0) ;                          SC  48:  2512
    LINE(LAMB,FINU,NMAX+1,TRY) ;                           SC  48:  2813
PLOT(LX+3,0,-3) ;                                          SC  48:  3113
END OF I LOOP ;                                            SC  48:  3412
END OF ABSORPTIVITY PLOT ROUTINE ;                         SC  48:  3712
                                                           SC  48:  3912
END;                                                       SC  48:  4113
                                             48 IS   49 LONG, NEXT SEG  31
                                                           SC  31: 45610
                                             31 IS  459 LONG, NEXT SEG  30



ENDJEND;

                                                           SC  30:  1810
PLOT(0,0,0,0,1J);                            30 IS   21 LONG, NEXT SEG  27
END;                                         27 IS  260 LONG, NEXT SEG   3
                                                           SC  31:  4810
END.                                                       SC  31:  4911
                                              3 IS   93 LONG, NEXT SEG   2
                                                           SC  21:   110
COS             IS SEGMENT NUMBER 0052, PRT ADDRESS IS 0160  2 IS  5 LONG, NEXT SEG  1
EXP                              0053               0174
LN                               0054               0173
SIN                              0055               0161
SQRT                             0056               0456
OUTPUT(W)                        0057               0133
BLOCK CONTROL                    0058               0005
INPUT(W)                         0059               0201
X TO THE I                       0060               0175
GO TO SOLVER                     0061               0245
ALGOL WRITE                      0062               0014
ALGOL READ                       0063               0015
ALGOL SELECT                     0064               0016
NUMBER OF ERRORS DETECTED =   0
PRT SIZE = 348; TOTAL PGM SEGM SIZE =  2978 WORDS; DISK SIZE = 160 SEGS; NO  PGM. SEGS =  55   LAST CARD WITH ERROR HAS SEQ #
ESTIMATED CORE STORAGE REQUIREMENT =  7265 WORDS.
14:10:58 THURSDAY, MAY 11, 1967     PROCESSOR TIME = 66.73 SECONDS    I/O TIME = 79.40 SECONDS
```

APPENDIX D

WHITTAKER AND GAMMA FUNCTIONS - DESCRIPTION OF TWO ALGOL PROCEDURES

By G. Basi
Computer Sciences R & D

ABSTRACT

This report describes the development and testing of two computer algorithms WOG and GAMMAC required in connection with computation of spectral properties of plasma arcs being carried out for Dr. C. H. Church of Quantum Electronics R & D. The algorithm WOG computes the irregular Whittaker function $W_{\eta,\ell+1/2}$ for real positive non-integral η, and for ℓ a non-negative integer. GAMMAC computes the function $\Gamma(z)$ for z real or complex. A very good accuracy has been obtained from both of these algorithms. GAMMAC is used in WOG, which calculates one of the four confluent hypergeometric functions needed in the calculation of transitions between eigenstates described by the Coulomb wave functions.

Summary

This report describes the development and testing of two computer algorithms WOG and GAMMAC required in connection with computation of spectral properties of plasma arcs being carried out for Dr. C. H. Church of Quantum Electronics R & D. The algorithm WOG computes the irregular Whittaker function $W_{\eta,\lambda+1/2}$ for real positive non-integral η, and for λ a non-negative integer. GAMMAC computes the function $\Gamma(z)$ for z real or complex. A very good accuracy has been obtained from both of these algorithms. GAMMAC is used in WOG, which calculates one of the four confluent hypergeometric functions needed in the calculation of transitions between eigenstates described by the Coulomb wave functions.

Introduction

Purpose of this study was to translate two subroutines WOG and GAMMAC from fortran into Algol and improve upon them. As received neither of the subroutines were in usable form, and considerable revision has been necessary. These algorithms will be used in a program to calculate the transitions between the eigenstates described by the Coulomb wave function.

The calculation of the transitions involves the use of confluent hypergeometric functions. Two of the four confluent hypergeometric functions are the solutions to Kummer's equation[1]

$$x \frac{d^2y}{dx^2} + (b-x) \frac{dy}{dx} - ay = 0.$$

The two solutions of the above are Kummer's functions ${}_1F_1(a; b; x)$ and $U(a; b; x)$ defined as follows:

$$y = {}_1F_1(a; b; x) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} \frac{x^n}{n!}$$

Where $(a)n = a(a+1) \ldots (a+n-1)$ for $n \geq 1$ and $(a)_o = 1$

$(b)n$ is similarly defined.

$$y = U(a;\ b;\ x) = \frac{\pi}{\sin \pi b} \left(\frac{{}_1F_1(a;\ b;\ x)}{\Gamma(1+a-b)\Gamma(b)} - \frac{x^{1-b}\ {}_1F_1(1+a-b;2-b;x)}{\Gamma(a)\Gamma(2-b)} \right) .$$

The other two confluent hypergeometric functions are the solutions to Whittaker's equation[2]

$$\frac{d^2y}{dz^2} + \left(-\frac{1}{4} + \frac{\eta}{z} - \frac{\ell^2+\ell}{z^2} \right) y = 0 .$$

Two solutions are Whittaker's functions $M_{\eta, \ell+1/2}(z)$ and $W_{\eta, \ell+1/2}(z)$. Whittaker's functions are defined as follows:

$$M_{\eta, \ell+1/2}(z) = z^{\ell+1} e^{-1/2z}\ {}_1F_1(\ell+1-\eta;2\ell+2:z).$$

$$W_{\eta, \ell+1/2}(z) = \frac{\pi}{\sin(2\ell+1)\pi} \left[\frac{-M_{\eta, \ell+1/2}(z)}{\Gamma(-\ell-\eta)\Gamma(2\ell+2)} + \frac{M_{\eta,-(\ell+1/2)}(z)}{\Gamma(\ell+1-\eta)\Gamma(-2\ell)} \right]$$

1.1 Available programs

Two programs that calculate the generalized hypergeometric function

${}_pF_q(a_1, a_2, \ldots a_p;\ b_1, b_2, \ldots b_q; z)$ are available in Algol B5000.

These programs were written by Hammers[3]. One of these two programs computes a general hypergeometric function which has a complex or real argument and any number of real parameters. The other program computes the same function for any number of real or complex parameters.

There are three programs called BEAUTY, BEAST, and CHIC in Fortran II. These programs were written by Johnson and Sangren[4] and calculate any generalized hypergeometric functions. Program BEAUTY can be used to calculate any generalized hypergeometric function with up to ten numerator and ten denominator parameters and one argument. Program BEAST can be used to compute analytical continuation of an ordinary hypergeometric function. The program called CHIC can be used for calculating 34 distinct hypergeometric series in two variables.

Two other programs WOG and HLIGAM are obtained from McGuire[5]. Both these programs were obtained in Fortran. Program WOG calculates the irregular Whittaker function $W_{\eta,\ell+1/2}(z)$ for $\eta>0$, real, and non-integral. Program HLIGAM calculates the same function where η is a pure imaginary number.

Both of these programs call for another program--GAMMAC-- which calculates the function $\Gamma(z)$ for any z real or comples. GAMMAC was obtained in Fortran from Dr. Mcguire.

2. Computation of GAMMAC

Procedure GAMMAC computes the value of $\Gamma(z)$ in the following way:

Let $z = (x,y)$ $\{$i.e. $z = x+iy\}$. The notation $z_i = (x_i,y_i)$ will be used during the discussion and shall be understood for $i = 1,2,3,4$. $\bar{z}$ will denote the complex conjugate of any complex number z.

For positive real integral values of z, $\Gamma(z)$ is computed as $(z-1)!$, for non-positive real integral values of z, the procedure does not work. If $x<0$, then the procedure uses the following recurrence relation to relate $\Gamma(z)$ to $\Gamma(z_1)$ where the real part of z_1 is positive.

$$\Gamma(z) = \frac{1}{z}\Gamma(z+1)$$

or

$$\Gamma(x,y) = \frac{1}{(x,y)}\ \Gamma(x+1,y).$$

Now if y_1 (which is the same as y), in z_1 is negative, the $\Gamma(z_1)$ is related to $\Gamma(z_2)$, where y_2 is positive, by the following relation

$$\Gamma(z_1) = \overline{\Gamma(\bar{z}_1)} = \overline{\Gamma(z_2)}$$

i.e. $z_2 = \bar{z}_1$, or $y_2 = -y_1$ and $x_2 = x_1$

with the use of the above relations the computation of $\Gamma(z)$ for general z reduces to the computation of $\Gamma(z_2)$ whose both real and imaginary parts are positive.

The next step is to relate $\Gamma(z_2)$ with $\Gamma(z_3)$ where $0 \leq y_3 < 1$. This is done by making use of Gauss' multiplication theorem. Gauss' multiplication theorem asserts that if $z_2 = nz_3$ where n is an integer then

$$\Gamma(z_2) = \frac{\Gamma(z_3)\Gamma(z_3+\frac{1}{n})\Gamma(z_3+\frac{2}{n}) \quad \ldots\ldots \Gamma(z_3+\frac{n-1}{n})}{(2\pi)^{\frac{1}{2}(n-1)}\, n^{\frac{1}{2}-z_2}}$$

In our case integer n is chosen to be the next greater integer than y_2 so that $y_2/n = y_3 < 1$. Next we relate $\Gamma(z_3)$ to $\Gamma(z_4)$ where z_4 is such that both x_4 and y_4 satisfy the inequalities $0 < x_4 \leq 1$, $0 \leq y_4 < 1$. In fact $y_4 = y_3$ and $x_4 = x_3 - [x_3]$ in case x_3 is a nonintegral real number and if x_3 is an integer $x_4 = 1$. where $[x_3]$ is greatest integer contained in x_3. The relation between $\Gamma(x_3)$ and $\Gamma(z_4)$ can conveniently be expressed as follows.

$$\Gamma(x_3) = (z_3-1)(z_3-2)(z_3-3) \ldots\ldots (z_4)\Gamma(z_4)$$

Now the computation of $\Gamma(z)$ for any complex number z has been related to $\Gamma(z_4)$ where z_4 is such that $0 < x_4 \leq 1$, $0 \leq y_4 < 1$. $\Gamma(z_4)$ is determined by the Padé power approximation of $1/\Gamma(z)$.

The procedure GAMMAC was obtained in Fortran and has been translated into Algol. Some changes were made during the translation to make the program

more efficient and clear. A basic constant was defined to greater accuracy to reduce the error. At present it is as discussed above, and calculates the function $\Gamma(z)$ for z real or complex. The values were checked against the available tables and found to be accurate to eight significant figures in the region

$$x = -2.0\ (.25)\ \ 2.0$$

$$y = -2.0\ (.25)\ -\ 2.5 \quad \text{and}$$

$$y = .25\ (.25)\ \ 2.0$$

3. Computation of Irregular Whittaker Function $W_{\eta,\ell+1/2}(z)$ for η real, positive and non-integral.

Program WOG calculates the irregular Whittaker function $\frac{W_{\eta,\ell+1/2}(z)}{\Gamma(\eta+\ell+1)}$ for η real, positive and non-integral. The function is computed by two different expressions for smaller and larger values of $2R/_{\eta}$ where $2R/_{\eta} = z$. The expression used to compute the function for small values of z is given by Hartree[6] and is as follows.

$$(-)^{\ell+1}\ \frac{W_{\eta,\ell+1/2}(z)}{\eta^{\ell}\Gamma(\eta-\ell)} = \frac{\sin \pi\eta}{\pi}\ e^{-1/2z}\ (\eta z)^{-\ell}$$

$$\left[-\sum_{m=0}^{2\ell} \frac{\Gamma(\eta+\ell+1)}{\Gamma(\eta+\ell+1-m)} \frac{(2\ell-m)!}{m!} z^{m} \right.$$

$$+ \sum_{m=2\ell+1}^{\infty} (-)^{m-1} \frac{\Gamma(\eta+\ell+1)}{\Gamma(\eta+\ell+1-m)} \frac{z^{m}}{m!(m-2\ell-1)!}$$

$$\left. \left\{ \log z + \pi \cot \pi\eta + \psi(\eta+\ell+1-m) - \psi(m+1) - \psi(m-2\ell) \right\} \right] \qquad (1)$$

Some important aspects of the evaluation of this expression are worth mentioning. Computation of the multiplying factor makes use of the identity

$$\frac{1}{\eta^{2\ell+1}} \quad \frac{\Gamma(\eta+\ell+1)}{\Gamma(\eta-\ell)} = \prod_{k=1}^{\ell} \left\{ 1-\left(\frac{k}{\eta}\right)^2 \right\} \qquad (A2)$$

In computing the finite sum in Equation (1), use is made of the identity

$$\prod_{k=1}^{m} \left[\frac{(\eta+\ell+1-k)}{k(2\ell+1-k)} \left(\frac{2R}{\eta}\right) \right] = \frac{\Gamma(\eta+\ell+1)}{\Gamma(\eta+\ell+1-m)} \frac{(2\ell-m)\,!}{m!(2\ell)\,!} z^m \qquad (A5)$$

In summing the infinite series in Equation (1) the summation parameter is transformed by $k = m - 2\ell - 1$ where k goes from 0 to ∞. The term when $k = 0$ is obtained separately. The expression containing ψ functions is computed in three different ways depending upon the value of η. In case $\eta < \ell$ and $\eta < 60$ the identities

$$\psi(n) = -\gamma + \sum_{k=1}^{n-1} \frac{1}{k} \qquad (n \geq 2) \qquad (2)$$

$$\psi(1+z) = -\gamma + \sum_{k=1}^{\infty} \frac{z}{k(k+z)} \qquad z \neq -1, -2, -3, \ldots\ldots (3)$$

$$\psi(1-z) = \psi(z) + \pi \operatorname{Cot} \pi z \qquad (4)$$

are used. If $\ell < \eta < 60$ the following additional relation is used,

$$\psi(n+z) = \frac{1}{(n-1)+z} + \frac{1}{(n-2)+z} + \ldots\ldots + \frac{1}{z} + \psi(z) \qquad (5)$$

In the case $\eta > 60$ the asymptotic expansion of the ψ function is used,

$$\psi(z) \sim \ln(z) - \frac{1}{2z} - \frac{1}{12z^2} + \frac{1}{120z^4} - \frac{1}{252z^6} + \cdots \quad .$$

$$(z \to \infty \text{ in } |\arg z| < \pi). \tag{6}$$

When the argument z of the Whittaker function is large, the asymptotic expansion is used for the computation in place of Equation (1). This expansion is given by Whittaker and Watson[8].

$$W_{\eta,\ell+1/2}(z) \sim e^{-\frac{1}{2}z} z^{\eta} \left\{ 1 + \sum_{n=1}^{\infty} \frac{\left\{(\ell+1/2)^2-(\eta-1/2)^2\right\}\left\{(\ell+1/2)^2-(\eta-3/2)^2\right\}\cdots}{\eta!\ z^{\eta}} \right.$$
$$\left. \left\{\frac{(\ell+1/2)^2-(\eta-n+1/2)}{n!\ z^n}\right\} \right\} \tag{7}$$

Some test runs with McGuire's program gave results of rather low accuracy--two or three significant figures, and some steps were taken to improve this. The major source of error appeared to be the summation for the ψ function in Equation (3), which is slowly convergent. McGuire truncated this summation at 50 terms. We have summed greater numbers of terms and also introduced a correction for the remainder term by consideration of the integral

$$\int_{x_0}^{\infty} \frac{dx}{x(x+a)} = \frac{1}{a} \ln\left(\frac{x_0}{x_0-a}\right)$$

By approximating to the integral in two different ways, we determine the error bounds for the remainder

$$\frac{1}{a}\ln\left|\frac{N-1}{N-1-a}\right| - \frac{1}{2(N-1)(N-1-a)} < \sum_{j=N}^{\infty} \frac{1}{j(j+a)} < \frac{1}{a} \ln\left|\frac{N-1/2}{N-1/2-a}\right|$$

The remainder term is approximated by the mean of the two bounds and good accuracy is obtained by taking N = 1001. In the case of the infinite sum involved

in (1), the series was being truncated when the term became less than 10^{-3} of the sum. In the modified version, the summation is truncated when the term becomes smaller than 10^{-8} of the sum and when at least 10 terms have been summed.

In computing the asymptotic expansion of Whittaker's function, the number of terms summed by McGuire was the greatest integer contained in $\ell + \eta$. The reason for this choice is not clear and it was found that improvement could be obtained by summing up to, but excluding, the smallest term (normal procedure with an asymptotic series). This method was, therefore, adopted.

With these modifications, a considerable increase in accuracy has been obtained, at the expense of some increase in computer time. Tables of the Whittaker's irregular function were not available. For checking the accuracy of the results Coulomb tables[7] were used. Coulomb tables list the functions $P_\ell(\frac{1}{\eta^2},R)$ and $Q_\ell(\frac{1}{\eta^2},R)$. The relation between Whittaker's function and the functions $P_\ell(\frac{1}{\eta^2},R)$ and $Q(\frac{1}{\eta^2},R)$ is given by the equation

$$W_{\eta,\ell+\frac{1}{2}}\left(\frac{2R}{\eta}\right) = \frac{\left(\frac{-2}{i}\right)^{\ell+1}\Gamma(\ell+\eta+1)}{(2\ell+1)!}\left\{Q_\ell(\tfrac{1}{\eta^2},R)\,\mathrm{Sin}\pi\eta + P_\ell(\tfrac{1}{\eta^2},R)\,\mathrm{Cos}\pi\eta\right\}$$

The results of the program have been found to agree with the results obtained by using the tabulated values to six or more significant figures for the ranges $\ell = 0, 1, 2$, $1/\eta^2 = -2.0(.2)-.2$, $z = .5(.5)4.0$. From results obtained in these ranges, it appeared appropriate to switch the computation from the series (1) to the asymptotic form (7) at the value $z = 9$.

Our next step in the project of writing a computer program for the calculation of transitions between eigenstates will be to check the results for the other program called HLIGAM against the available Coulomb tables and make the possible changes if necessary to improve its accuracy. Procedure HLIGAM calculates the function

$$\frac{(i\eta)^{\ell+1}}{\Gamma(\ell+1+i\eta)}\, W_{i\eta,\,\ell+1/2}\left(\frac{2R}{i\eta}\right)$$

for $i\eta$ a pure imaginary number. Then both of these functions (one calculated by WOG and the other by HLIGAM) will be integrated to determine the transitions probabilities. The result of integration will be checked against the tables given by Peach[9].

References

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9. G. Peach "A Revised General Formula for the Calculation of Atomic Photoionization Cross-sections", Private Communication (to be published in Memoirs of the R.A.S.).

Appendix Program Usage

A1. GAMMAC (x,y,u,v); An algol procedure to compute $\Gamma(z)$ for real or complex values of the argument z.

Procedure GAMMAC (x,y,u,v) computes the function $\Gamma(z)$ for any argument z, real or complex. This procedure can be included in any main program by including the following two cards in the programe declarations

```
$$ A GAMMAC
COMMENT HIGHER SEQUENCE CARD;
```

Both the cards must have some sequence number in the column 73-80. and the sequence number on the comment card must be higher than that on the $$ A GAMMAC card. The formal parameters x and y are the input parameters. x and y are both real and respectively are the real and imaginary part of the complex number z, whose gamma function is required. u and v are the output parameters and respectively are the real and imaginary parts of the complex number $\Gamma(z)$.

For example if one wants to calculate $\Gamma(z_1)$ and store the value at z_2 where $z_i = (x_i,y_i)$ for i = 1,2, are complex numbers then one would do so by including a card, at the desired place, in the main program with the following information on it.

GAMMAC (x_1,y_1,x_2,y_2);

Either one or both of the input parameters x and y can be real valued aritnmetic expressions. There is no loss of efficiency caused by using the expression as an actual input parameter since it is called by value.

Limitations. The procedure has the following limitations.

For the non-positive integral values of the argument an error message of divide by zero would occur since the gamma function is singular at such points. For the rest of the negative real values of the argument procedure calculates $\Gamma(z)$ except very close to the negative integers where an exponent overflow message would occur. For positive real values of the argument procedure computes $\Gamma(z)$ for $z \leq 53.3$. For larger values of z an error message of exponent overflow occurs. For very small values of z ($z < 8.758$ @-47) an error message of divide by zero occurs since computer sets such numbers to zero.

For pure imaginary argument $|z| > 66.$ the value of $|\Gamma(z)|$ is so small that it is set to zero by the computer.

For z = a complex number on the digonal x = y or x = -y and $x > 0$. While computing $\Gamma(z)$ of z such that $x > 42.00$ an error message of maximum argument of exponent would occur. On the diagonals x = y and x = -y for $x < 0$ the value of $\Gamma(z)$ is so small for $x < -22.60$ that it is set to zero by the computer.

A2. WOG (L, ETA, R, W); An algol procedure to compute the irregular Whittaker function $\frac{W_{\eta,\ell+1/2}(\frac{2R}{\eta})}{\Gamma(\eta+\ell+1)}$

The procedure WOG(L,ETA,R,W) calculates the function

$$\frac{W_{\eta,\ell+1/2}(\frac{2R}{\eta})}{\Gamma(\eta+\ell+1)}$$

A deck of cards for this procedure, to be included in the main program, may be obtained from the writer. The formal parameters L, ETA and R correspond to the variables ℓ, η and R in the Whittaker function $W_{\eta,\ell+1/2}(\frac{2R}{\eta})$ Either one or any number of these input variables L, ETA, and R can be a real valued arithmetic expression. There is no loss of efficiency caused by using an expression as an actual parameter since it is called by value. W is the output parameter, which has the value of the function $\frac{W_{\eta,\ell+1/2}(\frac{2R}{\eta})}{\Gamma(\eta+\ell+1)}$ as computed by the procedure.

One of the infinite series involved in computation is a function of ℓ and η but not R. This summation is the most time-consuming part of the computation. To increase efficiency when successive values of W are to be calculated with constant ℓ and η, varying R, the procedure has been written so that this particular sum is preserved between calls. It is recomputed only when either ℓ or η changes. Therefore it is recommended that the user arrange his program so that consecutive calls on the procedure WOG are made, as far as possible, with constant ℓ and η (i.e. variation of R should be the innermost loop).

Limitations. This procedure is limited to the real values of R, to η positive and nonintegral, and to ℓ integral only.

```
BEGIN                                                                           SC  21   010
                                                              START OF SEGMENT ********** 0002
                                                                                SC  21   010
COMMENT THIS PROGRAM IS WRITEN ONLY TO TEST THE ACCURACY OF THE                 SC  21   010
     PROCEDURE  GAMMAC.  PROCEDURE  GAMMAC CALCULATES THE GAMMA FUNCTION        SC  21   010
     OF A REAL OR COMPLEX ARGUMENT Z.  LN ( GAMMA(Z)) IS CALCULATED IN          SC  21   010
     THE MAIN PROGRAM AND THE VALUES ARE COMPARED WITH THE VALUES OF            SC  21   010
     LN( GAMMA(Z)) TABULATED IN HANDBOOK OF MATHEMATICAL FUNCTIONS,AMS 55       SC  21   010
     G. S. RASI;                                                                SC  21   010
FILE IN READER (2,10);                                                          SC  21   010
FILE OUT PRINTER 4(2,15);                                                       SC  21   312
INTEGER K,J;                                                                    SC  21   710
REAL X,Y,U,V,W,T;                                                               SC  21   710
     REAL FI,REL,IMAG;                                                          SC  21   710
     REAL ARRAY YI[0:20];                                                       SC  21   710
     FORMAT H1 (X5,"X",X5,"Y",X8,"COMPUTED VALUES OF LN(GAMMA(X,Y))",           SC  21   813
                                                              START OF SEGMENT ********** 0003
          X17,"TABULATED VALUES OF LN(GAMMA(X,Y))");                            SC  31   813
                                                              0003 IS 0021 LONG, NEXT SEG 0002
     FORMAT H2 (X12,2(X8,"REAL",X19,"IMAGINARY",X8 ));                          SC  21   813
                                                              START OF SEGMENT ** ******* 0004
                                                              0004 IS 0012 LONG, NEXT SEG 0002
     FORMAT F1 (X2,2F5.1, 4E23.11);                                             SC  21   813
                                                              START OF SEGMENT ********** 0005
                                                              0005 IS 0006 LONG, NEXT SEG 0002
PROCEDURE GAMMA2(X,Y,U,V);                                                      SC  21   813
     VALUE X,Y;                                                                 SC  21   813
     REAL X,Y,U,V;                                                              SC  21   813
     BEGIN                                                                      SC  21   813
          COMMENT THIS PROCEDURE CALCULATES GAMMA(X+IY) WHERE X AND Y ARE       SC  21   813
          NOT GREATER THAN ONE BY PADE POWER APPROXIMATION OF 1/GAMMA(Z);       SC  21   813
          REAL ARRAY A,B[0:9] ;                                                 SC  21   813
                                                              START OF SEGMENT ********** 0006
          INTEGER I;                                                            SC  61   210
          REAL E,F,G,H,P,Q,W;                                                   SC  61   210
          FILL A[*] WITH  0,0,1,1.2536302998,6.2294126804@-2,                   SC  61   210
                                                              START OF SEGMENT ********** 0007
              -1.9367439706@-1,9.5294069001@-3,1.0021677762@-2,                 SC  61   313
              -1.7669240217@-3,7.9027635693@-5;                                 SC  61   313
                                                              0007 IS 0010 LONG, NEXT SEG 0006
          FILL B[*] WITH 0,1,6.7641403695@-1, 3.2773507466@-1,                  SC  61   313
                                                              START OF SEGMENT ********** 0008
              1.0279994520@-1,2,7018504538@-2,5.1047208257@-3,                  SC  61   512



              8,7521995448@-4,9.5129148083@-5,6.0642802410@-6;                  SC  61   512
                                                              0008 IS 0010 LONG, NEXT SEG 0006
          E ← A[9]×X+A[8];                                                      SC  61   512
          F ← A[9]×Y;                                                           SC  61   713
          G ← B[9]×X+B[8];                                                      SC  61   911
          H ← B[9]×Y;                                                           SC  61   1112
          FOR I←7 STEP -1 UNTIL 1 DO                                            SC  61   1310
          BEGIN                                                                 SC  61   1410
               P ← E×X-F×Y;                                                     SC  61   1810
               F ← E×Y+F×X;                                                     SC  61   1811
               E ← P+A[I];                                                      SC  61   1812
               Q ← G×X-H×Y;                                                     SC  61   2010
               H← G×Y+H×X;                                                      SC  61   2211
               G← Q+B[I];                                                       SC  61   2412
          END;                                                                  SC  61   2610
          W ← E*2+F*2;                                                          SC  61   2811
          U ← (G×E+H×F)/W;                                                      SC  61   3012
          V ← (E×H-G×F)/W;                                                      SC  61   3312
     END;                                                                       SC  61   3612
                                                              0006 IS 0043 LONG, NEXT SEG 0002
PROCEDURE GAMMA1(X,Y,U,V);                                                      SC  21   813
     VALUE X,Y;                                                                 SC  21   813
     REAL X,Y,U,V;                                                              SC  21   813
     BEGIN                                                                      SC  21   813
          COMMENT  TO CALCULATE GAMMA(X+IY),WHERE X IS POSITIVE AND Y IS        SC  21   813
          LESS THAN 1;                                                          SC  21   813
          INTEGER N,J;                                                          SC  21   813
                                                              START OF SEGMENT ********** 0009
          REAL P;                                                               SC  91   010
          LABEL EXIT;                                                           SC  91   010
          IF X≤1 THEN BEGIN                                                     SC  91   010
          GAMMA2(X,Y,U,V);                                                      SC  91   111
          GO  TO EXIT;  END;                                                    SC  91   311
          N ← ENTIER (X);                                                       SC  91   313
          X ← X-N;                                                              SC  91   510
          IF X=0 THEN BEGIN                                                     SC  91   813
          N ←N-1; X ← 1; END;                                                   SC  91   810
          GAMMA2(X,Y,U,V);                                                      SC  91   1010
          N ← N-1;                                                              SC  91   1210
          FOR J ← 0 STEP 1 UNTIL N DO                                           SC  91   1311
          BEGIN                                                                 SC  91   1510
          P ← (X+J)×U-Y×V;                                                      SC  91   1510
          V ←(X+J)×V+Y×U;                                                       SC  91   1713
          U ← P;                                                                SC  91   2013
          END;                                                                  SC  91   2113
```

```
        EXIT;
     END,                                                              SC    9:  2410
                                                                       SC    9:  2410
  PROCEDURE GAMMAP(X,Y,U,V);                       0009 IS 0027 LONG, NEXT SEG 0002
     VALUE X,Y;                                                        SC   2:    813
     REAL X,Y,U,V;                                                     SC   2:    813
     BEGIN                                                             SC   2:    813
        COMMENT THIS PROCEDURE CALCULATES GAMMA(X+IY) WHEN X IS POSITIVE SC 2:    813
         IF Y IS POSITIVE THEN IT CALCULATES GAMMA OF THE NUMBER ITSELF SC  2:    813
        ELSE IT CALCULATES THE GAMMA OF THE CONJUGATE NUMBER AND TAKES  SC   2:    813
        THE CONJUGATE OF THAT;                                         SC   2:    813
        REAL A1,A2,XR,XI,C1,C2,C3,C4,C5,C,D,S,T,R;                     SC   2:    813
                                                                       SC   2:    813
        INTEGER I,J,K;                             START OF SEGMENT ********** 0010
     BOOLEAN BOOL;                                                     SC  10:    010
        LABEL EXIT;                                                    SC  10:    010
                                                                       SC  10:    010
        R ← 2.5066282746;                                              SC  10:    010
        IF Y ≥ 0 THEN BOOL ← TRUE ELSE BEGIN BOOL ←FALSE; Y ← (-Y); END; SC 10:   010
        IF Y ≤ 1 THEN BEGIN                                            SC  10:    013
        GAMMAI(X,Y,U,V);                                               SC  10:    613
        GO TO EXIT; END;                                               SC  10:    810
        J ← 1 + 1 + ENTIER (Y);                                        SC  10:   1010
        XR← X/J;                                                       SC  10:   1012
        XI← Y/J;                                                       SC  10:   1311
        GAMMAI(XR,XI,S,T);                                             SC  10:   1412
        A1 ← 1/J;                                                      SC  10:   1513
        FOR K←1 STEP 1 UNTIL J DO                                      SC  10:   1711
        BEGIN                                                          SC  10:   1812
           XR ← XR+A1;                                                 SC  10:   2110
           GAMMAI(XR,XI,U,V);                                          SC  10:   2110
           A2 ← S×U-T×V;                                               SC  10:   2211
           T  ← S×V+T×U;                                               SC  10:   2411
           S  ← A2;                                                    SC  10:   2612
        END;                                                           SC  10:   2613
        C1 ← R×J×SQRT(J) ;                                             SC  10:   2912
        C2 ← LN(J);                                                    SC  10:   3113
        C3 ← X×C2;                                                     SC  10:   3512
        C4 ← Y×C2;                                                     SC  10:   3613
        C5 ← EXP(C3)/C1;                                               SC  10:   3610
        C  ← C5×COS(C4);                                               SC  10:   3911
        D  ← C5×SIN(C4);                                               SC  10:   4110
        A2 ← C×S-D×T;                                                  SC  10:   4213
        V  ← C×T+D×S;                                                  SC  10:   4612
        IF NOT BOOL THEN  V ← (-V);                                    SC  10:   4613
                                                                       SC  10:   4911

        U  ← A2;
        EXIT:                                                          SC  10:   5112
     END;                                                              SC  10:   5212
                                                                       SC  10:   5310
  PROCEDURE GAMMAC(X,Y,R,I);                       0010 IS 00A0 LONG, NEXT SEG 0002
     VALUE X,Y;                                                        SC   2:    813
     REAL X,Y,R,I;                                                     SC   2:    813
     BEGIN                                                             SC   2:    813
                                                                       SC   2:    813
     COMMENT THIS PROCEDURE CALCULATES THE GAMMA FUNCTION OF A REAL OR SC   2:    813
        COMPLEX ARGUMENT Z = X + IY. X AND Y  RESPECTIVELY ARE THE REAL SC  2:    813
        AND IMAGINARY PARTS OF THE  ARGUMENT.  THE QUANTITIES R AND I  SC   2:    813
        RESPECTIVELY  ARE THE REAL AND IMAGINARY PART OF THE  VALUE OF SC   2:    813
        THE FUNCTION.  THIS PROCEDURE CALLS FOR ANOTHER PROCEDURE      SC   2:    813
        GAMMAP WHICH MUST ALSO BE INCLUDED IN THE MAIN PROGRAM;        SC   2:    813
                                                                       SC   2:    813
        REAL A, W,S,T,P,RE ;                                           SC   2:    813
                                                                       SC   2:    813
        INTEGER K,J,N;                             START OF SEGMENT ********** 0011
        LABEL EXIT;                                                    SC  11:    010
  IF Y = 0 THEN IF X MOD 1 = 0 THEN                                    SC  11:    010
  BEGIN                                                                SC  11:    010
     IF X ≤ 0 THEN R ← 1/0 ELSE                                        SC  11:    212
        BEGIN                                                          SC  11:    310
           A ← 1;                                                      SC  11:    513
           FOR K ← X-1 STEP -1 UNTIL 1 DO                              SC  11:    611
           A ← A × K;                                                  SC  11:    710
        END;                                                           SC  11:   1111
        R ← A;                                                         SC  11:   1110
        I ← 0;                                                         SC  11:   1310
        GO TO EXIT;                                                    SC  11:   1410
  END;                                                                 SC  11:   1510
        IF X ≥ 1 THEN BEGIN GAMMAP(X,Y,R,I); GO TO EXIT; END;          SC  11:     12
        N ← SIGN(1-X)×ENTIER(ABS(1-X));                                SC  11:     12
        A ← N+X;                                                       SC  11:    911
        GAMMAP(A,Y,R,I);                                               SC  11:   2412
        J ← N-1;                                                       SC  11:   2513
        FOR K ← 0 STEP 1 UNTIL J DO                                    SC  11:   2713
        BEGIN                                                          SC  11:   2910
           A ← X+K;                                                    SC  11:   3110
           W ← A*2+Y*2;                                                SC  11:   3110
           RE←(A×R+Y×I)/W;                                             SC  11:   3211
           I ←(A×I-Y×R)/W;                                             SC  11:   3412
           R ← RE;                                                     SC  11:   3711
        END;                                                           SC  11:   4011
                                                                       SC  11:   4111
```

```
        EXIT;                                                                              SC   11:  4312
        END;                                                                               SC   11:  4410
                                                                      0011 IS 0049 LONG, NEXT SEG 0002
        WRITE(PRINTER [DBL]);                                                              SC   21:   813
        WRITE(PRINTER [DBL]);                                                              SC   21:  1112
        WRITE(PRINTER[DBL],H1);                                                            SC   21:  1411
        WRITE(PRINTER[DBL],H2);                                                            SC   21:  1711
        PI ← 3.141592653;                                                                  SC   21:  2011
    FILL VECT WITH 0, 1.6,5.6,7.2,4,6,2.8,6.8,3.2,4.8,1.6,8.0,2.4,4.0,3.2,                 SC   21:  2110
                                                                      START OF SEGMENT ********** 0012
            4,4,6,4,8,0,1,4,9,4,7,2,8,8;                                                   SC   21:  2213
                                                                      0012 IS 0021 LONG, NEXT SEG 0002
        J ← 0;                                                                             SC   21:  2213
        FOR X ← 1.0,1.0,1.1,1.1,1.2,1.2,1.3,1.3,1.4,1.4,1.5,1.5,1.6,1.6,                   SC   21:  2312
                1.7,1.7,1.8,1.8,1.9,1.9 DO                                                 SC   21:  5510
        BEGIN                                                                              SC   21:  6410
        J ← J+1;                                                                           SC   21:  6410
        Y ← Y[J];                                                                          SC   21:  7011
            GAMMA(X,Y,U,V);                                                                SC   21:  7111
            R ← LN(SQRT(U*2+V*2));                                                         SC   21:  7213
            T ← ARCTAN(V/U);                                                               SC   21:  7610
            IF U<0 THEN IF V>0 THEN T ← T+PI;                                              SC   21:  7713
            IF T > 0 THEN IF V<0 THEN T ← T-PI;                                            SC   21:  8112
            READ (REALER,/,REL,IMAG);                                                      SC   21:  8511
    FOR K←1 STEP 1 WHILE IMAG≥PI DO                                                        SC   21: 10813
            IMAG ← IMAG - 2×PI;                                                            SC   21: 11110
            WRITE ( PRINTER,F1,X,Y,R,T,REL,IMAG);                                          SC   21: 11311
        END;                                                                               SC   21: 12911
    END.                                                                                   SC   21: 12913
                                                                      0002 IS 0133 LONG, NEXT SEG 0001
   ARCTAN          IS SEGMENT NUMBER 0013, PRT ADDRESS IS 0043
   COS                               0014                  0055
   EXP                               0015                  0052
   LN                                0016                  0051
   SIN                               0017                  0054
   SQRT                              0018                  0050
   OUTPUT(W)                         0019                  0041
   BLOCK CONTROL                     0020                  0005
   INPUT(W)                          0021                  0047
   X TO THE I                        0022                  0053
   ALGOL WRITE                       0023                  0014
   ALGOL READ                        0024                  0015
   ALGOL SELECT                      0025                  0016
NUMBER OF ERRORS DETECTED = 000                      LAST CARD WITH ERROR HAS SEQ #
PRT SIZE=0059;    TOTAL SEGMENT SIZE=00463 WORDS;    DISK STORAGE REQ.=00541 WORDS;    NO. SEGS.=0026.



ESTIMATED CORE STORAGE REQUIREMENT = 02440 WORDS.
15:34:39 FRIDAY, APRIL 14, 1967    PROCESSING TIME = 11.70 SECONDS    I/O TIME = 21.42 SECONDS
```

X	Y	COMPUTED VALUES OF LN(GAMMA(X,Y,)) REAL	IMAGINARY	TABULATED VALUES OF LN(GAMMA(X,Y,)) REAL	IMAGINARY
1.0	1.5	-1.353312251653+00	-1.15444794288E-01	-1.3593122658478+00	-1.15-48793558E-01
1.0	5.4	-7.1951175924098+00	-1.3551911229470+00	-7.[illegible]18.3759500E+00	-1.[illegible]31113990E+00
1.1	7.2	-7.2[illegible]133733478+00	1.4539581542038+00	-9.2361133035700+00	1.[illegible]58110200E+00
1.1	9.4	-1.2883529843348+01	4.7442119371898-01	-1.2883528000008+01	4.7442119401888-01
1.2	2.1	-2.23375548815[illegible]+00	7.151123314908-01	-2.2332554844830E+00	7.1411231110E-01
1.2	6.3	-7.43118652023[illegible]+00	2.4191411158082-01	-7.8380452050008+00	2.6441411287088-01
1.3	3.2	-3.172-18433548+00	1.5923018[illegible]+00	-3.1720154107508+00	1.[illegible]1812A[illegible]E+00
1.3	4.8	-5.363735747983+00	-2.355088547548+00	-5.363735741558+00	-2.35[illegible]85485A8+00
1.4	1.4	-1.13733587303A+00	3.4425533178128-01	-1.1303356742998+00	3.4425533370238-01
1.4	8.[illegible]	-0.778A,3552[illegible]+00	-2.5623025043068+00	-0.7746235881098+00	-2.54[illegible]9748[illegible]E+00
1.5	2.[illegible]	-1.95530091507E+00	1.0848743143708+00	-1.7542608158088+00	1.0[illegible]1763370A8+00
1.5	4.[illegible]	-3.9[illegible]20031998+00	3.0020742103408+00	-3.970200310608+00	3.0[illegible]7421152A8+00
1.6	3.2	-2.5112651958118+00	2.3741126847E+00	-2.9112451953588+00	2.0741324817A8+00
1.6	6.4	-7.1875529[illegible]E+00	8.3723794444088-01	-7.[illegible]870520059008+00	5.37[illegible]7930840E-01
1.7	4.8	-4.7243285400448+00	-1.8201637035E+00	-4.725,2858078E+00	-1.8001437040198+00
1.7	8.0	-9.1883984171[illegible]+00	-2.1303503140E+00	-9.1483983422008+00	-2.0313513702608+00
1.8	1.4	-4.751158487[illegible]-01	7.2370742853OE-01	-4.75111458 0A08-01	7.2[illegible]0032971088-[illegible]
1.8	9.4	-1.12170087[illegible]+01	1.5051211152908+00	-1.121773090008+01	1.5[illegible]1011704538+00
1.9	7.2	-7.0134455174[illegible]+00	2.7994281049508+00	-7.4128455172098+00	2.7274247208E+00
1.9	8.5	-0.85429143091[illegible]+00	-1.3571810584034-01	-0.854201444508+00	-1.35[illegible]5133738A-01

LABEL 000000000R2-15TF0001A7104? COMPILE GAMMATEST/GOST

DA010034 GAMMA

APPENDIX E

RADIATIVE TRANSPORT IN A XENON ARC

by

B. W. Swanson

I. INTRODUCTION

The problem of interest has been to determine the steady state temperature profile in a Xenon arc, which requires a solution of the energy equation

$$\frac{\partial^2 S}{\partial r^2} + \frac{1}{r}\frac{\partial S}{\partial r} - \vec{\nabla} \cdot \vec{F} + \sigma(P,S)E^2 = 0 \qquad (1)$$

where $\vec{F}(r)$ is the radiative flux vector, T the plasma temperature, σ the electrical conductivity, P the pressure and E the electric field. The Schmitz function S is defined by the equation

$$S(T) = \int_{TW}^{T} K(T)dT \qquad (2)$$

and the divergence of F is given by

$$\vec{\nabla} \cdot \vec{F} = \frac{dF}{dr} + \frac{F}{r} \qquad (3)$$

where the radiative flux F is found from the equation

$$F(r) = \int_0^{\infty} \int_{\omega=4\pi} I_\lambda(r,\vec{\omega})\vec{\omega}d\omega d\lambda \qquad (4)$$

In equation 4, $\vec{\omega}$ is a unit direction vector and $I_\lambda(r,\vec{\omega})$ is the monochromatic intensity of radiation.

The first phase of this program consisted of writing a computer program for calculating the radiative flux[1], which can be expressed as

$$F(r) = -4 \int_{\lambda min}^{\lambda max} \int_{o}^{\pi} \int_{o}^{R_M(\phi)} K_\lambda(s)\, B_\lambda(s)\, G_1[\beta_\lambda(s)] \cos\phi \; ds\, d\phi\, d\lambda \qquad (5)$$

In equation 5, $K_\lambda(T)$ is the spectral absorptivity, λmin and λmax the wavelength band of interest, B_λ is the Planck function, $\beta_\lambda \equiv \int_o^s K_\lambda(\zeta)\, d\zeta$ and the function G is given by

$$G_n(x \int_{o}^{\frac{\pi}{2}} e^{-\frac{x}{\sin\theta}} (\sin\theta)^n \, d\theta \qquad (6)$$

and accounts for the attenuation of radiation by self absorption. The geometry for the evaluation of equation 5 is shown in figure 1.

Since the numerical evaluation of the triple flux integral is expensive the second phase of the program sought a faster flux approximation method. An analysis was made which permitted an a'priori integration with respect to wavelength to reduce computation time. The approximate flux integral is given[2] by the equation

$$\hat{F}(r) = -4 \int_{o}^{\pi} \int_{o}^{R_M(\phi)} K_a(s)\, B(s)\, G_1 \left[\int_{s}^{R_M(\phi)} K_a(\zeta)\, d\zeta \right] \cos\phi \; ds\, d\phi \qquad (7)$$

where

$$B(s) = \int_{\lambda_1}^{\lambda_2} B_\lambda[T(s)]\, d\lambda \qquad (8)$$

and the mean absorption coefficient $K_a(s)$ is defined by the equation

$$K_a(s) = \left[\frac{b}{b + \tau_P(s)}\right] \left[\frac{b + \tau_R(s)}{b + \tau_P(s)}\right] K_P(s) + \left[\frac{\tau_P(s)}{b + \tau_P(s)}\right] K_R(s) \qquad (9)$$

The term b in a constant of the order of unity which can be varied to improve the approximation. The terms τ_R and τ_P are the Rosseland and Planck optical lengths along the ray from point M to point R in figure 1 and are given by

$$\tau_R(s) = \int_0^s K_R(\zeta)d\zeta$$

$$\tau_P(s) = \int_0^s K_P(\zeta)d\zeta \qquad (10)$$

where the Planck and Rosseland absorption coefficients are given by

$$K_P(T) = \int_{\lambda_1}^{\lambda_2} \frac{K_\lambda(T)\ B_\lambda(T)d\lambda}{B(T)}$$

$$K_R^{-1}(T) = \int_{\lambda_1}^{\lambda_2} \frac{\frac{1}{K_\lambda(T)}\ \frac{dB_\lambda}{dT}\ d\lambda}{\frac{dB}{dT}} \qquad (11)$$

and

$$B(T) = \int_{\lambda_1}^{\lambda_2} B_\lambda(T)d\lambda \qquad (12)$$

The form of the approximation is such that under optically thin conditions when τ_P and τ_R are much less than unity, the mean absorption coefficient K_a approaches the Planck absorptivity K_P and equation 7 is exact. Under optically thick conditions, when τ_P and τ_R are much greater than unity, K_a approaches the Rosseland mean K_R and equation 7 is a good approximation.

The subject of this report, which is the third phase of the program, consists of the numerical solution of equation 1 utilizing the exact and approximate flux programs.

II. XENON PROPERTIES

The initial data needed for a numerical solution consists of the electrical conductivity, thermal conductivity and spectral absorptivity as functions of temperature and pressure. The temperature dependence of the S integral is shown in figure 2 for a pressure of 11 atmospheres, and the electrical conductivity σ is shown as a function of S in figure 3. The variation of spectral absorptivity with temperature is shown in Table I. An inspection of the table reveals that the spectral absorptivity in the ultra violet region is orders of magnitude greater than that in the visible region. Therefore, the flux computer program consists of an exact flux program for the U. V. and an approximate flux program for the visible. The wavelength bands defining these regions are given by the equations

$$\text{U.V.} \quad \begin{cases} \lambda\text{min} = .0612 \times 10^{-4} \text{ cm} \\ \text{max} = .0952 \times 10^{-4} \text{ cm} \end{cases}$$

$$\text{Visible} \quad \begin{cases} \lambda_1 = .1034 \times 10^{-4} \text{ cm} \\ \lambda_2 = 2.0 \times 10^{-4} \text{ cm} \end{cases}$$

III. NUMERICAL ANALYSIS

A steady state solution of the energy equation can be obtained by solving the "transient" equation

$$\frac{\partial S}{\partial t} = \frac{\partial^2 S}{dr^2} + \frac{1}{r}\frac{\partial S}{\partial r} - \left[\frac{dF}{dr} + \frac{F}{r}\right] + \sigma(s)E^2 \qquad (13)$$

until a steady state solution is achieved. The following calculation procedure was followed:

Table I - Spectral Absorptivity of Xenon (cm^{-1})

	$\lambda x10^4$ cm	T [°K] 3000	6000	10000	14000	18000
VISIBLE	2.0	1.257@-14	4.909@-05	.2502	3.046	2.406
	.7500	2.616@-14	1.679@-05	.0523	.5612	.4115
	.4615	1.224@-12	1.052@-04	.1352	.9441	.5476
	.3333	8.184@-12	9.594@-05	.0768	.5461	.3027
	.2609	6.775@-11	1.076@-04	.0511	.3594	.1872
	.2143	5.557@-10	1.194@-04	.0345	.2446	.1193
	.1818	9.842@-10	9.506@-05	.0225	.1598	.0761
	.1579	6.446@-10	6.226@-05	.0147	.1049	.0501
	.1395	4.449@-10	4.297@-05	.0107	.0725	.0347
	.1250	3.198@-10	3.089@-05	.00731	.0521	.0250
	.1132	2.376@-10	2.295@-05	.00543	.0387	.0186
	.1034	1.817@-10	1.751@-05	.00414	.0295	.0142
ULTRA VIOLET	.0952	2,269.0	1,134.0	614.1	145.9	13.07
	.0882	2,094.0	1,047.0	56..0	135.7	12.07
	.0822	1,920.0	959.7	519.8	124.4	11.07
	.0769	1,746.0	872.6	472.6	113.1	10.06
	.0723	1,572.0	785.5	425.4	101.8	9.06
	.0682	1,397.0	698.4	378.3	90.51	8.05
	.0645	1,223.0	611.3	331.1	79.22	7.05
	.0612	1,049.0	524.2	283.9	67.94	6.04

(a) specify arc radius and central core temperature.

(b) specify an initial temperature profile

(c) calculate a radial flux profile

(d) define E by the equation

$$E = \sqrt{\frac{-\nabla_r^2 S(o) + 2\frac{dF(o)}{dr}}{\sigma(o)}}$$

(e) select a time step Δt and solve for a new S profile

(f) repeat steps c,d, and e until the solution converges to a steady state

The field E is so defined as to keep the central temperature essentially constant. This procedure was adopted to avoid large central temperature variations which would greatly affect the flux and its divergence. The finite difference equation used to replace equation 13 is

$$\frac{S_i^{n+1} - S_i^n}{\Delta t} = \frac{1}{\Delta r^2}\left[\left(1 + \frac{\Delta r}{2r_i}\right)S_{i+1}^{n+1} + \left(1 - \frac{\Delta r}{2r_i}\right)S_{i-1}^{n+1} - 2S_i^{n+1}\right] - \left[\frac{F_{i+1}^n - F_{i-1}^n}{2\Delta r} + \frac{F_i^n}{r_i}\right] + \sigma(S_i^n)(E^n)^2 \tag{14}$$

where the subscript i denotes a radial position. Equation 14 is an implicit difference equation, which for linear equations, is known[3] to be unconditionally stable. Now let $\Theta = \frac{\Delta t}{\Delta r^2}$ and define the coefficients $C_{i,j}$ by the equations

$$C_{i,i-1} = -\Theta\left(1 - \frac{\Delta r}{2ri}\right)$$

$$C_{i,i} = (1 + 2\Theta) \tag{15}$$

$$C_{i,i+1} = -\Theta\left(1 + \frac{\Delta r}{2ri}\right)$$

Then equation 14 can be written as

$$C_{i,i-1}\, S_{i-1}^{n+1} + C_{i,i}\, S_i^{n+1}\, C_{i,i+1}^{n+1} = B_i^n \tag{16}$$

where

$$B_i^n \equiv \sigma(S_i^n)(E^{\cdot}, \quad ^2 - [\frac{F_{i+1}^n - F_{i-1}^n}{2\Delta r} + \frac{F_i^n}{r_i}] \tag{17}$$

Let $\vec{S}^n$ and $\vec{B}^n$ define the vectors

$$\vec{S}^n = \begin{pmatrix} S_1^n \\ S_2^n \\ \vdots \\ S_i^n \\ \vdots \\ S_N^n \end{pmatrix}; \quad \vec{B}^n = \begin{pmatrix} B_1^n \\ B_2^n \\ \vdots \\ B_i^n \\ \vdots \\ B_N^n \end{pmatrix} \tag{18}$$

Then the finite difference equations can be written in matrix form as

$$\langle C \rangle\, \vec{S}^{n+1} = \vec{B}^n \tag{19}$$

The k^{th} row of <C> contains only the coefficients $C_{K,K-1}$, $C_{K,K}$, $C_{K,K+1}$ and the matrix is tri- diagonal. The matrix <C> can be "inverted" very efficiently by Gaus's[4] elimination method. The first equation (i=1) is used to eliminate S_1^{n+1} from the second equation (i=2), the new second equation used to eliminate S_2^{n+1} from the third equation and so on until finally the new last but one equation can be used to eliminate S_{N-2}^{n+1} from the last equation, giving only one equation with only one unknown S_{N-1}^{n+1}. The unknowns S_{N-2}^{n+1}, S_{N-3}^{n+1},...S_1^{n+1} can then be found in turn by back substitution. The method provides a fast computational procedure for large numbers of equations. In the numerical solution,

50 radial increments were employed. The flux program was used to evaluate the flux at 9 points and intermediate values were obtained with the use of a quadratic interpolation program.

IV. NUMERICAL SOLUTIONS

Numerical solutions were obtained for a pressure of 11 atm. and central arc temperatures of 10,000°K and 18,000°K. For the first example, several iterative S profiles are shown in figure 4. S_o denotes the initial profile, and S_{29} denotes the final profile obtained after 29 time increments. The final solution has a maximum error ε of .03% where ε is defined as

$$\varepsilon = \frac{\frac{\partial S}{\partial t}}{\sigma E^2} \tag{20}$$

In figure 5 are shown several iterative flux profiles. For the final S profile (S_{29}), the approximate flux calculations were compared with exact calculations over the range λ_1-λ_2 and were found to agree to within 1%. In figure 6 is shown the final temperature profile corresponding to S_{29}. The temperature profile is very flat with a narrow conduction layer near the tube wall. The total current was evaluated from Ohm's law as

$$I = 2\pi E \int_o^R r\sigma[S(r)]dr \tag{21}$$

In figure 7 is given the variation of E with "time", showing a convergence to 20.69 volts/cm.

The iterative S profiles for the second example are shown in figure 8. A total of 80 time increments was required for convergence and the final profile S_{80} differs markedly from the initial S_o profile. The final solution S_{80} has a maximum error of 0.2%. In figure 9 are shown the initial and final flux profiles. A comparison of approximate and exact flux calculations over the range λ_1-λ_2 gave agreement to within

10%. Therefore the "final" solution S_{80} must still be considered an approximation to the exact solution. The temperature profile corresponding to S_{80} is shown in figure 10. Lowke and Capriotti[5] have shown that the curvature of the temperature in the central core region is due to self absorption effects. Also, the thermal conduction edge is smaller than in the first example. The iterative variation of E is given in figure 11 showing convergence to a final value of 68.95 volts/cm and the corresponding current is 5795 amps. In summary, these examples indicate that the numerical method employed is stable and provides a convenient method for obtaining steady state solutions to the energy equation. Furthermore, with slight modification, the method can be used to calculate actual thermal transients in radiative plasmas, for applications where transient effects are important.

ACKNOWLEDGEMENTS

The author gratefully acknowledges the assistance of Mr. R. Lieberman who modified and consolidated existing flux programs; Mr. B. Wang who programmed the finite difference equations; and discussions with Mr. J. Vine and Dr. J. Lowke.

NOMENCLATURE

B_λ Planck function $\beta_\lambda = \dfrac{2c^2h}{\lambda^5[\exp(\frac{ch}{\lambda KT})-1]}$

$B(T)$ $B(T) = \int_{\lambda_{min}}^{\lambda_{max}} B_\lambda(T)dT$

b constant in equation 9

B_i^n $B_i^n \equiv \sigma(S_i^n)(E^n)^2 - [\dfrac{F_{i+1}^n - F_{i-1}^n}{2\Delta r} + \dfrac{F_i^n}{r_i}]$

$\vec{B}^n$ $\vec{B}^n = \text{col}(B_1^n, B_2^n, \cdots B_i^n \cdots B_N^n)$

$C_{i,i-1} = -\Theta(1 + \dfrac{\Delta r}{2ri})$

C_{ij} $C_{i,i} = (1 + 2\Theta)$

$C_{i,i+1} = -\Theta(1 - \dfrac{\Delta r}{2ri})$

$< C >$ matrix $< C > = (C_{ij})$

E Electric Field (volts/cm)

E^n value of E for $n\Delta t$ (volts/cm)

$\vec{F}$ radiative flux vector (watt/cm^2)

$\vec{F} = \vec{r}\,F(r)$

$F(r)$ $\quad F(r) = \int_{\lambda_{min}}^{\lambda_{max}} \int_{\omega=4\pi} I_\lambda(r,\vec{\omega})\vec{\omega} d\omega d\lambda$; equation 5

$\hat{F}(r)$ approximate flux; see equation 7

$G_n(x)$ $\quad G_n(X) = \int_0^{\frac{\pi}{2}} e^{-\frac{x}{\sin\theta}} (\sin\theta)^n d\theta$

I current (amperes)

$I_\lambda(r,\vec{\omega})$ intensity of radiation at r in direction $\vec{\omega}$ (watts/cm^3)

$K(T)$ thermal conductivity (watt/$cm\,^oK$)

K_a mean absorption coefficient in equation 9 (cm^{-1})

K_R Rosseland mean absorption coefficient (cm^{-1})

$$K_R^{-1} = \int_{\lambda_1}^{\lambda_2} \frac{1}{K_\lambda} \frac{dB\lambda}{dT} d_\lambda / \frac{dB}{dT}$$

K_P Planck mean absorption coefficient (cm^{-1})

$$K_P = \int_{\lambda_1}^{\lambda_2} K_\lambda(T)\, B_\lambda(T) d\lambda / B(T)$$

N number of radial subdivisions

n number of "time" steps

P arc pressure (atm)

R	tube radius (cm)
r	radial coordinate (cm)
r_i	i^{th} radial position (cm)
Δr	$\Delta r = r_i - r_{i-1}$ (cm)
$S(T)$	$S = \int_{Tw}^{T} KdT$ (watt/cm)
s	position along a ray (cm)
S_i^n	value of $S(r_i)$ at the n^{th} time step
T	temperature (^oK)
T_w	wall temperature (^oK)
Δt	time step
β_λ	$\beta_\lambda = \int_o^S K_\lambda(\zeta)d\zeta$
Θ	$\Theta = \Delta t/\Delta r^2$
K_λ	spectral absorptivity (cm^{-1})
λ	wavelength (cm)
λ_1	$\lambda_1 = .1034 \times 10^{-4}$ cm
λ_2	$\lambda_2 = 2 \times 10^{-4}$ cm

λ_{min} $\lambda_{min} = .0612 \times 10^{-4}$ cm

λ_{max} $\lambda_{max} = .0952 \times 10^{-4}$ cm

σ electrical conductivity (mho/cm)

τ_R Rosseland optical length; $\tau_R = \int_o^S K_R(\zeta)d\zeta$

τ_p Planck optical length; $\tau_p = \int_o^S K_p(\zeta)d\zeta$

ϕ spherical coordinate measuring azimuth angle of a ray in figure 1.

$\vec{\omega}$ unit direction vector of a ray

REFERENCES

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3. R. D. Richtmyer, Difference Methods for Initial-Value Problems Interscience Publishers Inc., 1957.

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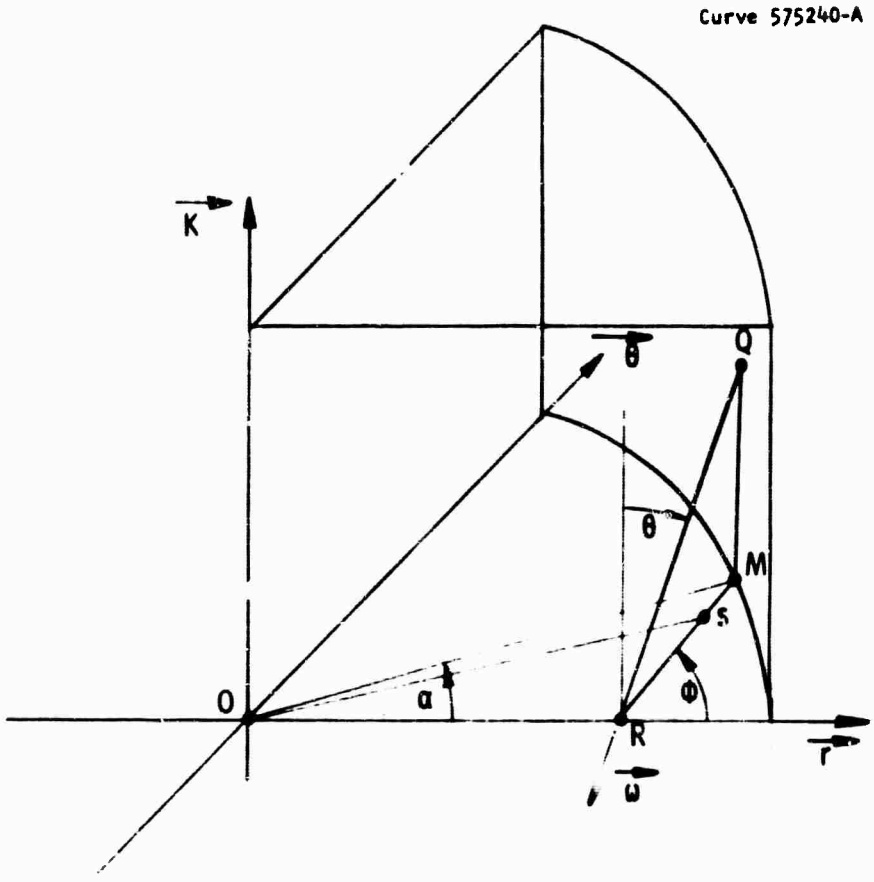

Fig. 1 – Arc geometry with $\theta' = 0$

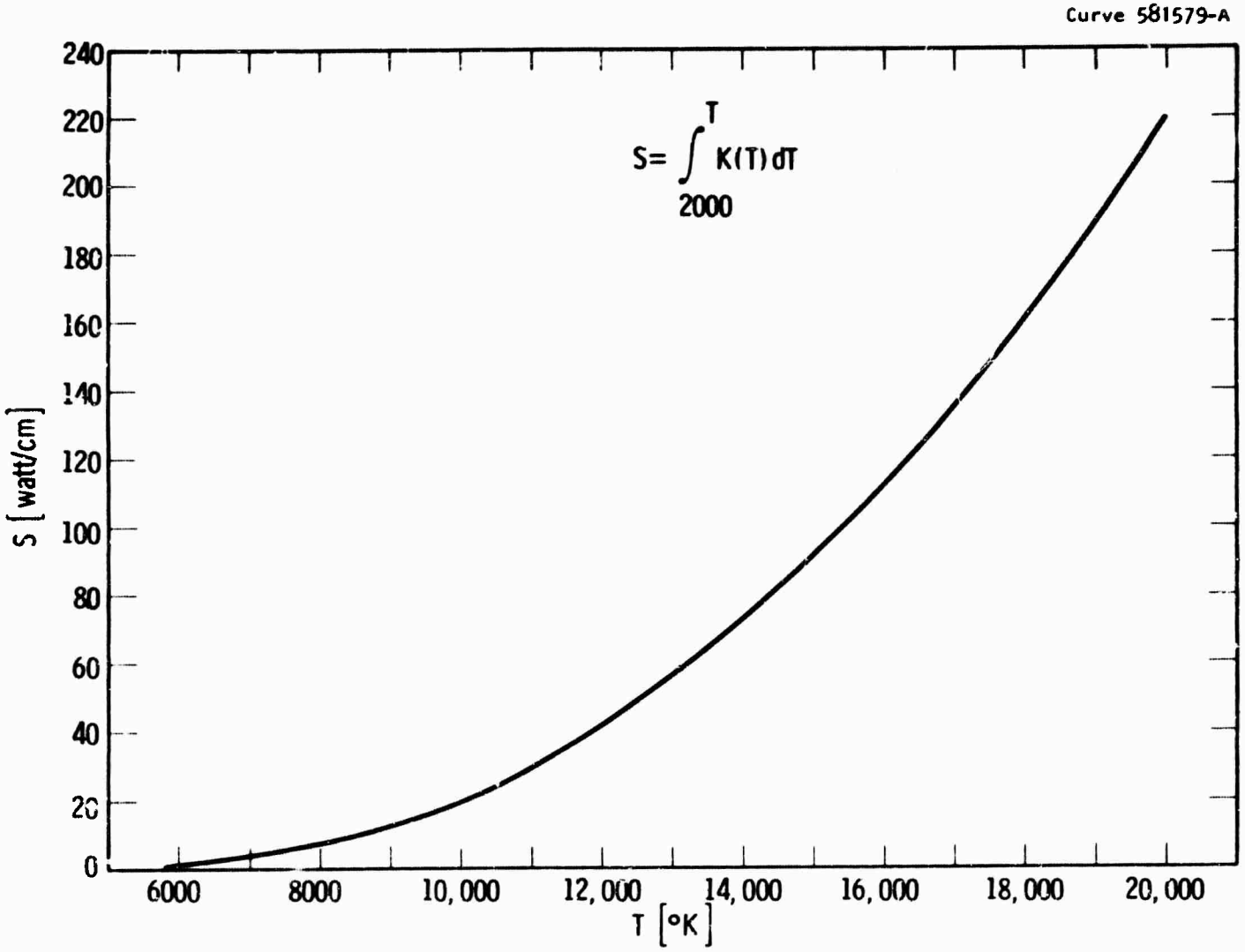

Fig. 2—S(T) vs T for Xenon at 11 atm pressure

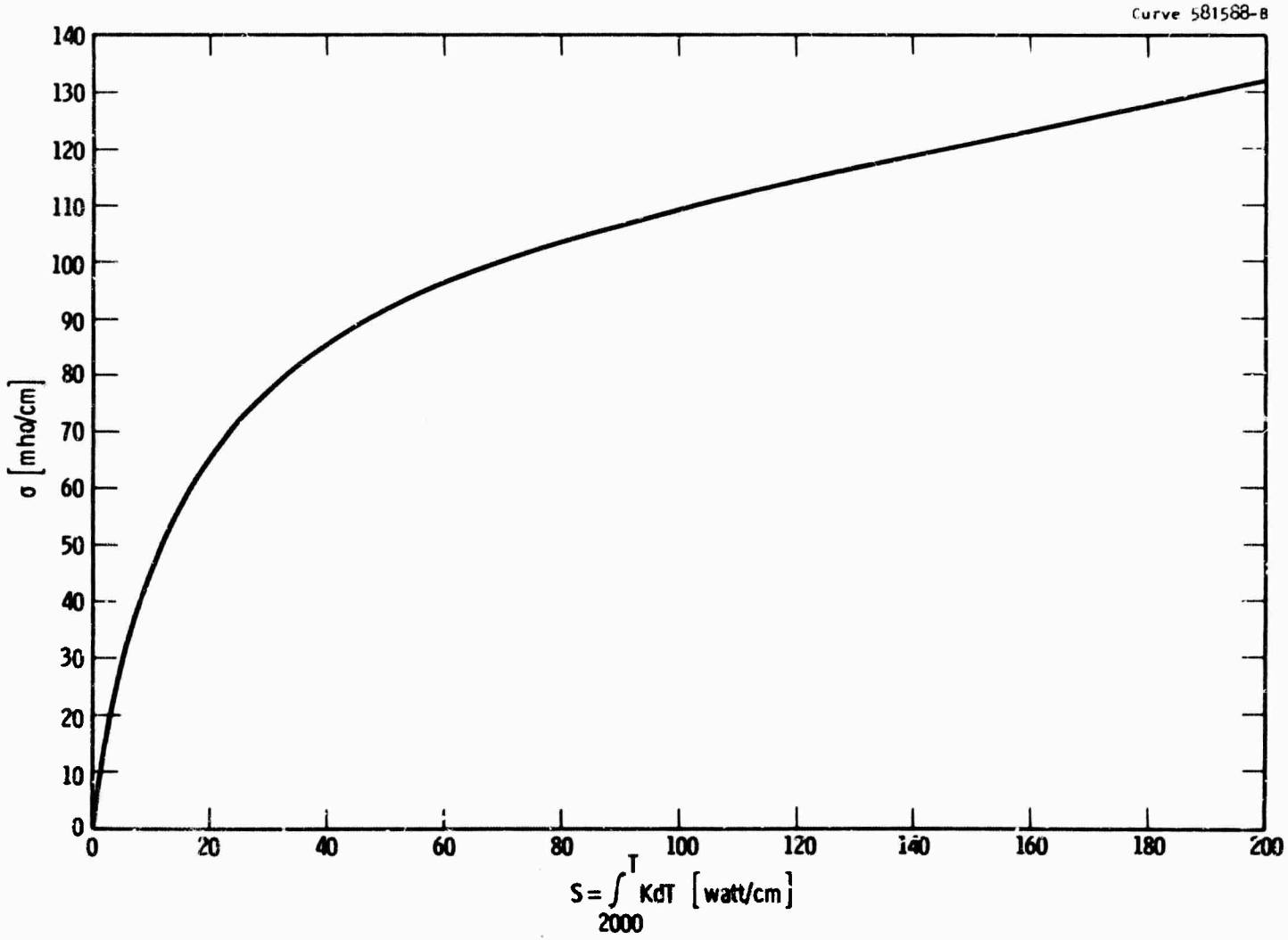

Fig. 3—σ vs S for Xenon at 11 atm pressure

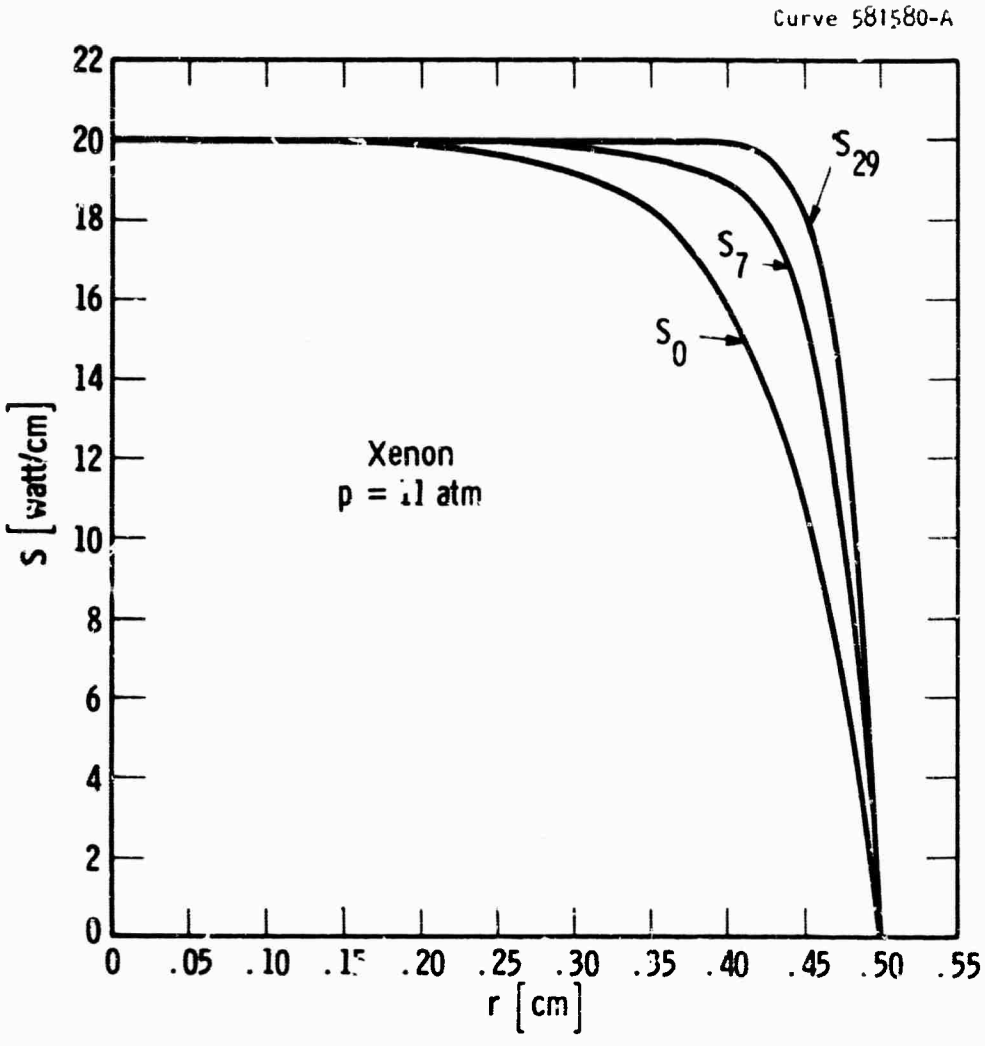

Fig. 4—Iterative S profiles

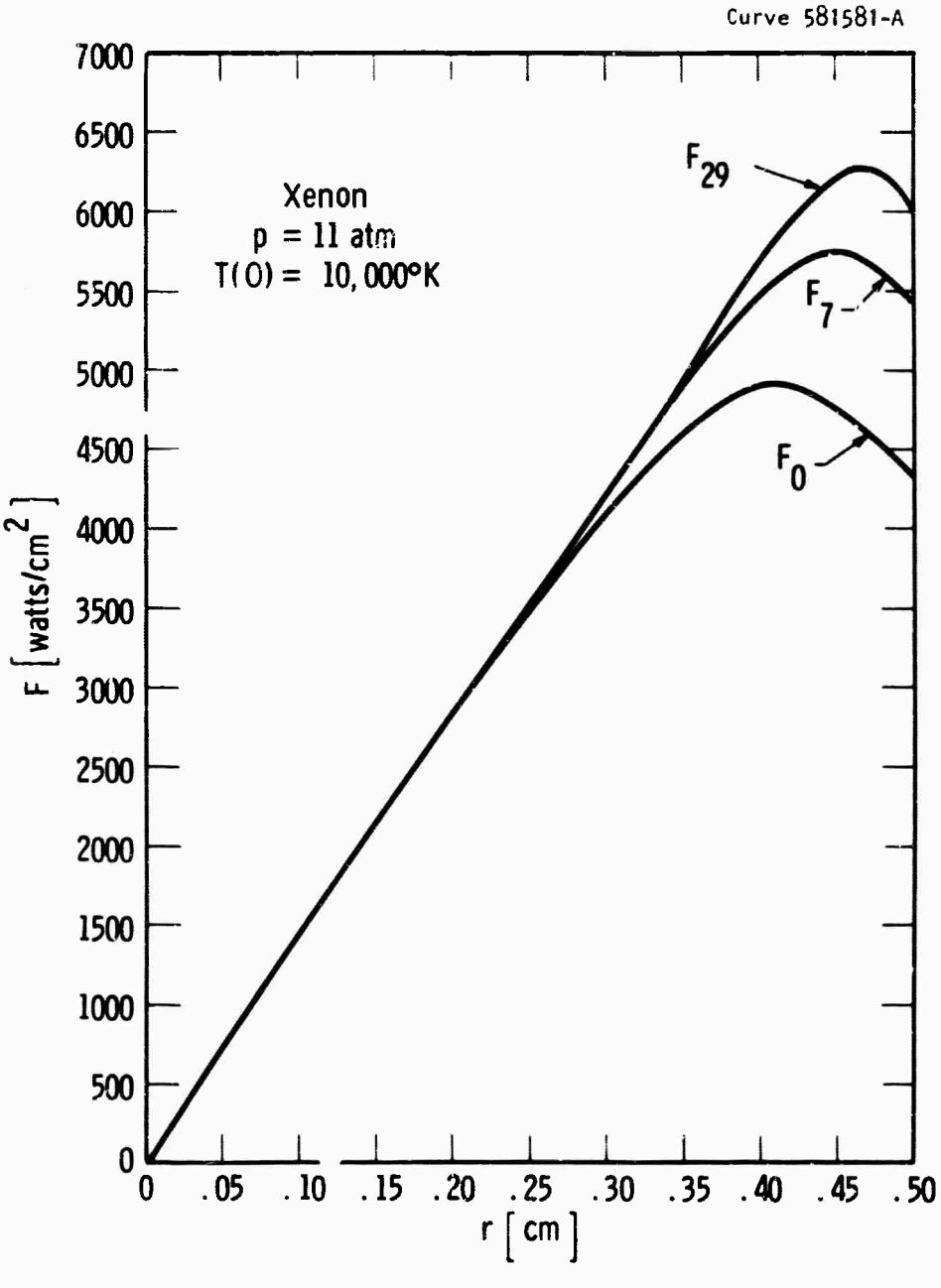

Fig. 5—Iterative flux profiles

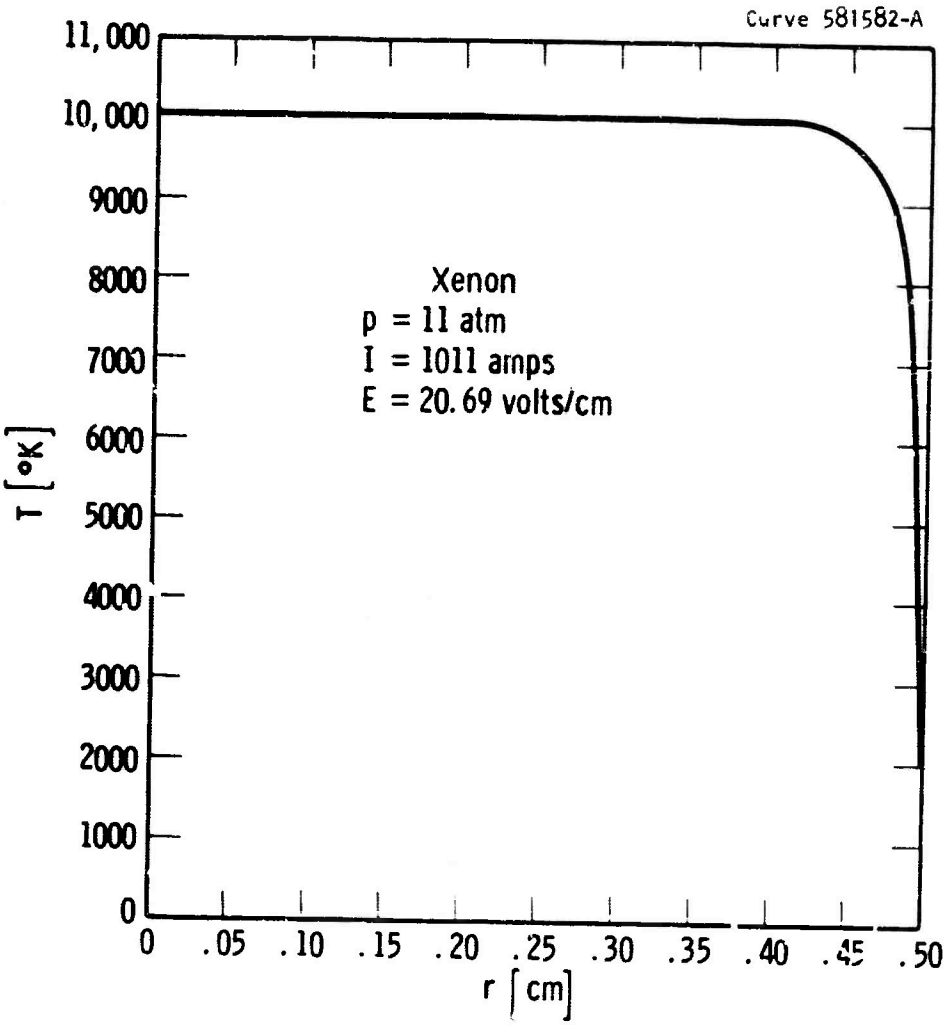

Fig. 6—Steady state temperature profile

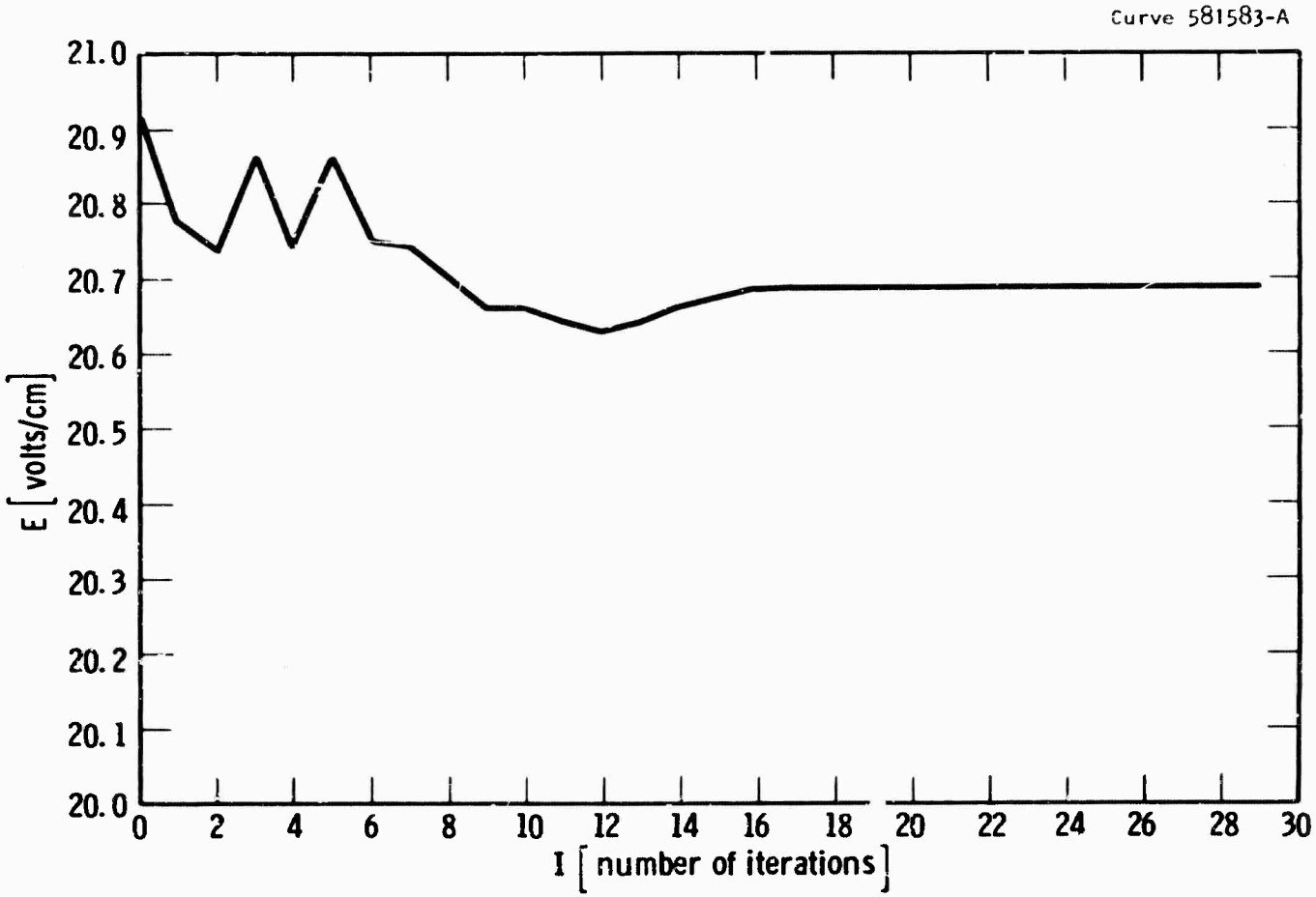

Fig. 7—Variation of E with iteration

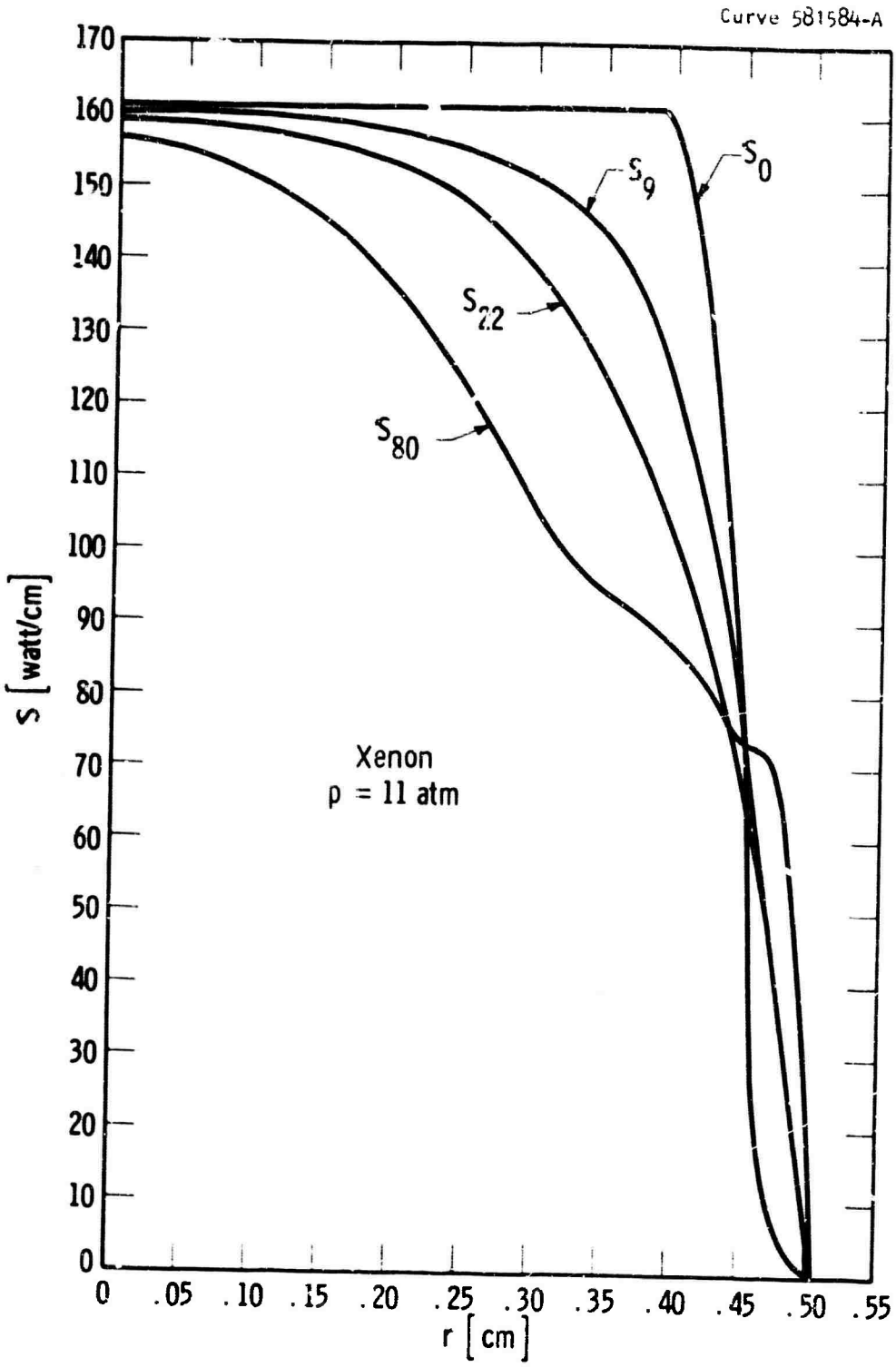

Fig. 8--Iterative S profiles

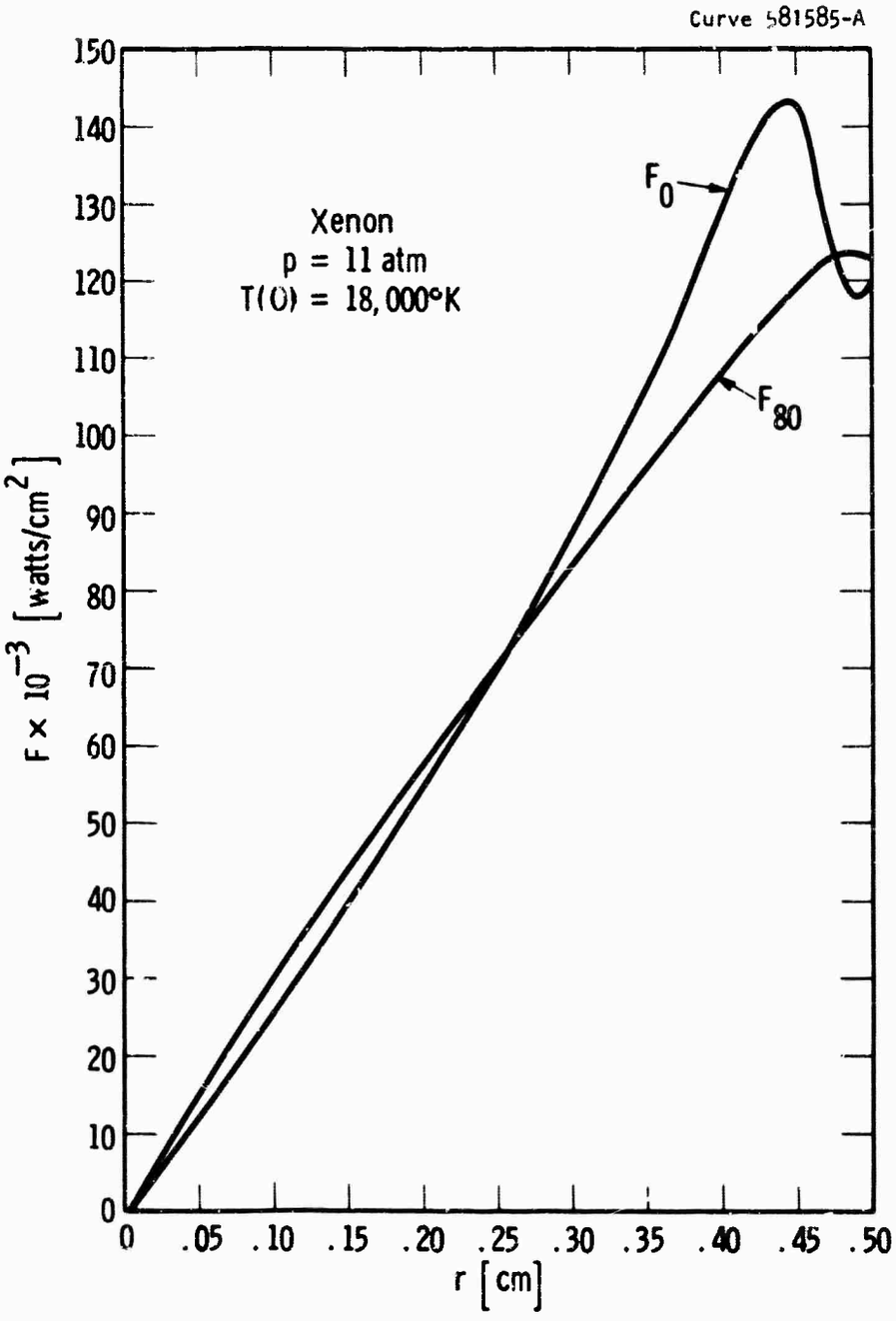

Fig. 9—Iterative flux profiles

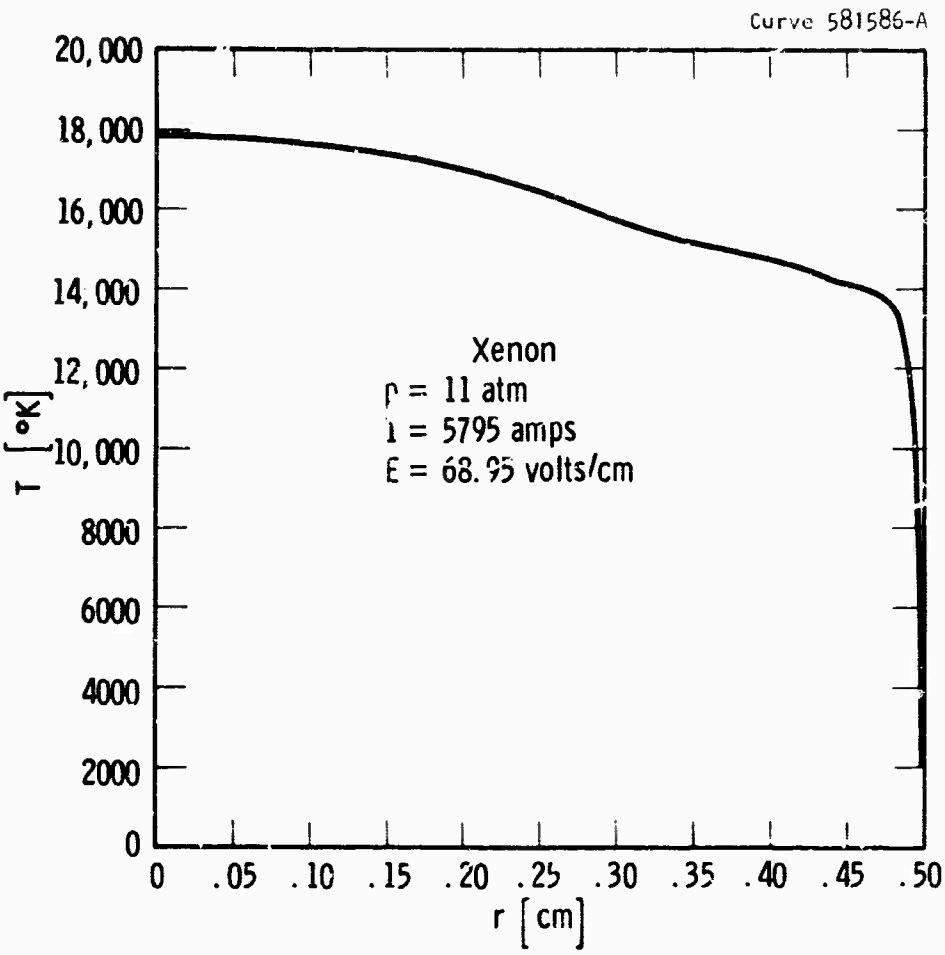

Fig. 10—Steady state temperature profile

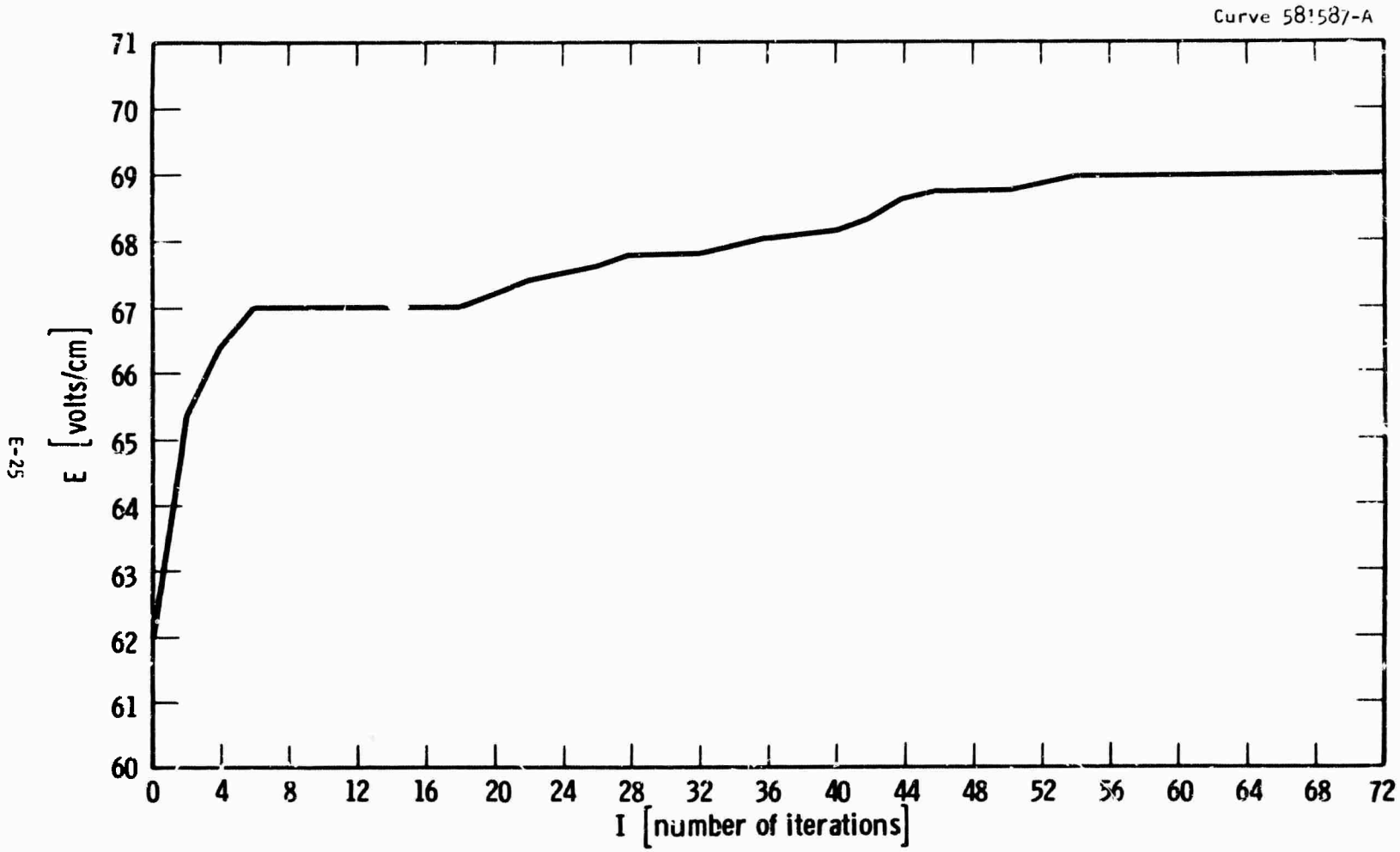

Fig. 11—Variation of E with iteration

```
BEGIN                                                                SC  21  010
                                                    START OF SEGMENT **********  2
COMMENT                                                              SC  21  010
THIS PROGRAM CALCULATES THE TEMPERATURE PROFILE OF AN ELECTRICAL     SC  21  010
ARC COLUMN HAVING CYLINDRICAL SHAPE AND INFINITE LENGTH AND POSSESSING SC 21 010
AXIMETRICAL SPATIAL VARIANCES ABOUT ITS AXIS. THE PROGRAM DETERMINES SC  21  010
THE PROFILE BY AN ITERATIVE PROCESS USING A TIME DEPENDENT DIFFERENTIAL SC 21 010
ENERGY BALANCE EQUATION WHICH INCLUDES MAC ACTIVE AS WELL AS THERMAL SC  21  010
TRANSPORT MECHANISMS .                                               SC  21  010
THE PROGRAM CONTAINS NINE READ STATEMENTS. THEY ARE LISTED BELOW IN  SC  21  010
ORDER OF CALL .                                                      SC  21  010
                        ( 1 )                                        SC  21  010
RB======(REAL) THE ARC COLUMN RADIUS  (UNITS== CM ) .                SC  21  010
N ======(INTEGER)  NUMBER OF STEPS IN R (RADIUS)                     SC  21  010
                        ( 2 )                                        SC  21  010
DT======(REAL )  TIME STEP SIZE  ( UNITS == SEC. ) .                 SC  21  010
NT======(INTEGER )  NUMBER OF TIME STEPS TO BE RUN                   SC  21  010
                        ( 3 )                                        SC  21  010
T ======(ARRAY )  INITIAL RADIAL TEMPERATURE PROFILE, CONTAINS 51 VALUES SC 21 010
                  STARTING WITH THE CENTRAL TEMPERATURE AND STEPPING IN SC 21 010
                  EQUAL INCREMENTS OF RADIUS TO RB  (UNITS==DEG. KELVIN ) SC 21 010
                        ( 4 )                                        SC  21  010

SI======( ARRAY )  AN ARRAY GIVING THE VALUES OF THE INTEGRAL OF     SC  21  010
                   THERMAL CONDUCTIVITY WITH RESPECT TO TEMPERATURE  SC  21  010
                   . UNITS== WATTS/CM ) .                            SC  21  010
SHY=====(ARRAY )  AN ARRAY OF ELECTRICAL CONDUCTIVITIES ( UNITS==MHOS/CM) SC 21 010
NOTE                                                                 SC  21  010
THE ABOVE TWO ARRAYS ARE READ IN SIMULTANEOUSLY AT CORRESPONDING     SC  21  010
TEMPERATURE VALUES .                                                 SC  21  010
                        ( 5 )                                        SC  21  010
NPMI===(INTEGER )  NUMBER OF  AYS IN MAKING NUMERICAL APPROXIMATIONS  SC  21  010
                   IN THE FLUX PROCEDURE ( USUALLY  AD IN AS SIX ) .  SC  21  010
APPROXCS==(REAL)  APPROXIMATE STEP SIZE TO BE TAKEN ALONG EACH OF THE SC 21 010
                  THE ABOVE RAYS (USUALLY READ IN AS .05 ) .         SC  21  010
                        ( 6 )                                        SC  21  010
RT======(REAL )  FIRST TEMPERATURE VALUE OF THE KAPPA TABLE DEFINED BELOW SC 21 010
DT======(REAL)  TEMPERATURE STEP SIZE OF KAPPA TABLE                 SC  21  010
FT======(REAL )  LAST TEMPERATURE VALUE OF THE KAPPA TABLE           SC  21  010
NOTE  THE ABOVE THREE TERMS HAVE UNITS OF DEG. KELVIN                SC  21  010
                        ( 7 )                                        SC  21  010
RFREQ==(REAL )  FIRST FREQUENCY VALUE OF THE KAPPA TABLE             SC  21  010
DFREQ==(REAL    FREQUENCY STEP SIZE OF THE KAPPA TABLE               SC  21  010
EFREQ==(REAL )  LAST FREQUENCY VALUE OF THE KAPPA TABLE              SC  21  010
J=======(INTEGER )  FREQUENCY INDEX        ( WITH 1  CORRESPONDING TO SC 21 010
                    RFREQ ) WHICH DEFINES THE SPECTRUMS TO BE USED IN SC 21 010
```

```
                  THE FLUX PROCEDURE FOR THE EXACT AND APPROXIMATE             SC   21   010
                  CALCULATIONS THEREIN , THE EXACT SOLUTION USES THE           SC   21   010
                  FREQUENCY SPECTRUM CORRESPONDING TO THE INDEXES  OF          SC   21   010
                  2 TO THAT FOR FFREQ ,                                        SC   21   010
NOTE THE UNITS OF FREQUENCY IS  CYCLES/SEC.                                    SC   21   010
                              ( A )                                            SC   21   010
KAPPA---(ARRAY )  SPECTRAL ABSORPTIVITY VALUES WHICH ARE A FUNCTION OF         SC   21   010
                TEMPERATURE AND FREQUENCY RESPECTIVELY ( UNITS  1/CM )         SC   21   010
                              ( B )                                            SC   21   010
BST----(REAL )  THE FIRST TEMPERATURE VALUE ( DEG. KELVIN )CORRESPONDING       SC   21   010
               TO THE FIRST ENTRY OF THE ST FUNCTION OF (3. ,                  SC   21   010
FNT----(REAL)  LAST TEMPERATURE VALUE CORRESPONDING TO LAST ENTRY OF ST        SC   21   010
DRT----(REAL )  THE TEMPERATURE INCREMENT OF THE ST FUNCTION .  ;              SC   21   010
FILE IN PASSG DISK SERIAL (1,330) ;                                            SC   21   010
FILE  IN  READER  (2, 10)  ;                                                   SC   21   312
FILE  OUT  PUNCH  D(2,10)  ;                                                   SC   21   710
FILE  OUT  PRINTER  4(2,15)   ;                                                SC   21  1012
LABEL  START, FIN, EXIT     ;                                                  SC   21  1410
REAL  RHO, LOA, BETA,  E, DL, DT, RB, DSMAX, E1, IFC              ;            SC   21  1410
ARRAY   S, A, B, C, SIGMA, F,OGV,R,Q,OS[0:55], TH[0:15] ,   SNY[0:90] ;        SC   21  1410
ARRAY  T, ST[0:95]  ;                                                          SC   21  2112
ARRAY  SC, OVGF, SFQ, SS[0:55]  ;                                              SC   21  2312
INTEGER  I, J, K, N  ,M , COUNT ,NN ,NT ;                                      SC   21  2610



DEFINE   SL = STEP  1 UNTIL  #   ;                                             SC   21  2610
COMMENT DARTIME;                                                      00000000 SL   21  2610
                                                                      ******** SC   21  2610
FORMAT  FMT1(X1, F5.2,R11.A,X2,R11.A,X1,R11.A,X3, F9.A,X3,R11.A,X3,            SC   21  2610
                                                     START OF SEGMENT **********     A
     R11.A, X3, R11.A,X3, R11.A) ,                                             SC   A1  2A10
        HD1(X", "R", X10, "S", X11,"F",X10,"T",X9,"SIGMA",X6,"COND PART"       SC   A1  2610
     ,X4, "OVGF",X11, "SUE+2", X8 ,"SUM RATE",/ )   ;                          SC   A1  2A10
                                                          A IS   74 LONG, NEXT SEG    2
REAL PROCEDURE ILAG ( X , XA , N , Y0 , DY ) ;                          ILAG       SC   21  2610
COMMENT ORDER 3 LAGRANGE INTERPOLATION, EQUAL DEPENDENT STEP, SINGLE    ILAG  2    SC   21  2610
INDEPENDENT , DEPENDENT VARIABLE, EXTRAPOLATES IF NOT XA[0]SXSXA[N] ,  ILAG  3    SC   21  2610
X  = DESIRED INDEPENDENT VALUE                                          ILAG  4    SC   21  2610
XA = NAME, INDEPENDENT VARIABLE VALUE TABLE (SINGLE SUBSCRIPT)          ILAG  5    SC   21  2610
N  = MAX INDEX OF XA TABLE ( ≥ 3 )                                      ILAG  6    SC   21  2A10
Y0 = FIRST DEPENDENT VALUE (REFERENCE POINT -- FOR XA[0] )              ILAG  7    SC   21  2610
DY = STEP SIZE, DEPENDENT VARIABLE ;                                    ILAG  8    SC   21  2A10
VALUE X, N, Y0, DY ; REAL X, Y0, DY ; INTEGER N ; ARRAY XA[0] ;         ILAG  9    SC   21  2610
     BEGIN INTEGER I ; REAL E0, E1, E2, E3, F10, F20, F31, F32, G ;     ILAG 10    SC   21  2A10
                                                     START OF SEGMENT **********     5
     E0 = SIGN( XA[N] - XA[0] ) ;                                       ILAG 11    SC   51   010
     FOR I = 0 STEP 1 WHILE (I+1)<N AND SIGN(X-XA[I+2])=E0 DO ;         ILAG 1     SC   51   312
     F10 = ( E1 * XA[ I + 1 ] - X ) - ( E0 * XA[I] - X ) ;              ILAG  3    SC   51  1310
```

```
    F20 ← ( E2 × XA[ I + 2 ] − X ) − E0 ;                              ILAG 11   SC   51   1711
    F31 ← ( E3 × XA[ I + 3 ] − X ) − E1 ;                              ILAG  5   SC   51   2011
    F32 ← E3 − E2 ;                                                    ILAG  6   SC   51   2311
    ILAG ← (( G + 1 × DY + Y0 ) × E3 / F10 / F20 − ( 3 × DY + 1 ) × E0  ILAG  7   SC   51   2412
        / F31 / F32 ) × E1 × E2 / ( E3 − E0 ) − (( DY + G ) × E2 / F10  ILAG  8   SC   51   2910
        / F31 − ( 2 × DY + G ) × E1 / F20 / F32 ) × E0 × E3 / ( E2 − E1 ILAG 10   SC   51   3410
END ILAG ;                                                             I  7      SC   51   3911
                                                   5 IS   46 LONG, NEXT SEG    2
REAL PROCEDURE LAG ( X , X0 , DX , Y , N ) ;                           LAG  1    SC   21   2610
COMMENT                                                                          SC   21   2610
X  = DESIRED INDEPENDENT VALUE                                         LAG  4    SC   21   2610
X0 = FIRST INDEPENDENT VALUE OF Y TABLE (FOR Y[0])                     LAG  5    SC   21   2610
DX = TABLE STEP FOR INDEPENDENT                                        LAG  6    SC   21   2610
Y  = NAME,DEPENDENT VARIABLE VALUE TABLE (MUST BE SINGLE SUBSCRIPT)    LAG  7    SC   21   2610
N  = MAX INDEX OF Y TABLE ( ≥ 4 ) ;                                    LAG  8    SC   21   2610
    VALUE X , X0 , DX , N ;                                            LAG  9    SC   21   2610
    REAL X , X0 , DX ; INTEGER N ; ARRAY  Y[0] ;                       LAG 10    SC   21   2610
    BEGIN                                                              LAG 11    SC   21   2610
        INTEGER I ; REAL S ;                                           LAG 12    SC   21   2610
                                                   START OF SEGMENT **********    6
Y←ENTIER(S←(X−X0)/DX);                                                           SC   61    010
IF S=I THEN LAG←Y[I] ELSE                                                        SC   61    311
LAG←(Y[I+1]−Y[I])    ×(S−I)+Y[I];                                                SC   61    512



    END LAG ;                                                          LAG 18    SC   61   1110
                                                   6 IS   14 LONG, NEXT SEG    2
        REAL PROCEDURE ULAG(X, XA, Y, N);                              00009200 SC   21   2610
COMMENT ORDER 3 LAGRANGE INTERPOLATION, NO EQUAL STEPS, SINGLE DEPENDENT 00009300 SC   21   2610
& INDEPENDENT VARIABLE, EXTRAPOLATES IF NOT XA[0] ≤ X < XA[N] .        00009400 SC   21   2610
X  = DESIRED INDEPENDENT VALUE                                         00009500 SC   21   2610
XA = NAME, INDEPENDENT VARIABLE VALUE TABLE (SINGLE SUBSCRIPT)         00009600 SC   21   2610
Y  = NAME, DEPENDENT VARIABLE VALUE TABLE (SINGLE SUBSCRIPT)           00009700 SC   21   2610
N  = MAX INDEX OF BOTH XA & Y TABLES ( ≥ 3 ) ;                         00009800 SC   21   2610
        VALUE X, N;                                                    00009900 SC   21   2610
        REAL X;                                                        00010000 SC   21   2610
        ARRAY XA, Y[0];                                                00010200 SC   21   2610
        INTEGER N;                                                     00010100 SC   21   2610
        BEGIN                                                          00010300 SC   21   2610
            INTEGER I;                                                 00010400 SC   21   2610
                                                   START OF SEGMENT **********    7
            REAL E0, E1, E2, E3, F10, F20, F31, F32;                   00010500 SC   71    010
            E0← SIGN(XA[N]−XA[0]);                                     00010600 SC   71    010
            FOR I← 0 STEP 1 WHILE(I< I)<ASS AND SIGN(X−XA[I+2])=E0 DO  00010700 SC   71    312
                ;                                                      00010800 SC   71   1212
            F10←(E1← XA[I+1]−X)−(E0← XA[I]−X);                         00010900 SC   71   1310
            F20←(E2← XA[I+2]−X)−E0;                                    00011000 SC   71   1711
            F31←(E3← XA[I+3]−X)−E1;                                    00011100 SC   71   2 11
```

```
        F32+ E3-E2)                                              00011200 SC   71   2311
        ULAW+(Y[I]*E3/F10/F20-Y[I+3]*E0/F31/F32)*E1*E2/(E3-E0)+(Y[I  00011300 SC   71   2A12
          +1]*E2/F10/F31-Y[I+2]*E1/F20/F32)*E0*E3/(E1-E2)        00011400 SC   71   3111
      END ULAW;                                                  00011500 SC   71   3713
                                                          7 IS   AA LONG, NEXT SEG    2
PROCEDURE FLUX(SP,FP,R) ;                                                 SC   21   2610
VALUE R ; REAL R ;                                                        SC   21   2610
ARRAY  SP,FP[0] ;                                                         SC   21   2610
COMMENT  PROCEDURE FOR EVALUATING FLUX GIVEN  S FUNCTION     ;            SC   21   2610
BEGIN                                                                     SC   21   2610
BOOLEAN   APPF  ;                                                         SC   21   2610
                                                   START OF SEGMENT **********    8
INTEGER N,J,PHI;                                                          SC   81   010
LABEL APPROX,EXACT,EXIT ;                                                 SC   81   010
REAL X,SUM',SUMS,A,B,TN,RSNXY,IBN, A,VN,LAMBDA,IRR,TEMP,YMT,XLN,          SC   81   010
     NPHI,IPHI,         K,KRINT,K2INT ;                                   SC   81   010
ARRAY FRX[0:12] ;                                                         SC   81   010
ARRAY RT,TP,FXPAPG[0:51]; ARRAY RT,TPI[0:12]  ;                           SC   81   113
OWN REAL BFREQ,EFREQ,DFREQ ;                                              SC   81   610
OWN REAL APPROXDS   ;                                                     SC   81   610
OWN REAL OPHI,Z,LAMMAX,BT,ET,DT,BKT,EKT,DKT,LITTLEP;                      SC   81   610
REAL O  ;                                                                 SC   81   610
OWN INTEGER NT,NKT ;                                                      SC   81   610


OWN ARRAY    LAM,DLAMBDA[0:190]  ;                                        SC   81   610
OWN ARRAY C,MS,US[0:11,0:10]  ;                                           SC   81   813
OWN ARRAY G[0:300],KAPPA[0:50,0:35],MAX[0:11]  ;                          SC   81   1912
OWN ARRAY                 RR[0:36],KK,KP[0:35] ;                          SC   81   1913
REAL TAUP2,TAUR2,KP2,KR2,TAUP,TAUP,COUNTS,KPT,KRT,TAUA,PRR ;              SC   81   2A13
IF COUNT >1 THEN GO EXACT ;                                               SC   81   2A13
READ(READER,/,NPHI,APPROXDS);                                             SC   81   2610
OPHI + 3.1A159265360/NPHI ; NPHI + 3.1A1592A536 - OPHI*,A  ;              SC   81   3613
READ(PASSG,301,G[*]) [EXIT] ;                                             SC   81   3913
READ(READER,/,BT,DT,ET)[EXIT] ; COMMENT TEMP AT WHICH KAPPA IS GIVEN ;    SC   81   AA11
READ(READER,/,BFREQ,DFREQ,EFREQ,Z )[EXIT] ;                               SC   81   5913
LAMMAX + (EFREQ-BFREQ)/DFREQ + 1 ;                                        SC   81   7A13
FOR N + 1 STEP 1 UNTIL LAMMAX DO LAM[N]+ 3P10/(BFREQ+(N-1)*DFREQ ) ;      SC   81   7710
NT +(ET-BT)/DT ;                                                          SC   81   8312
FOR N+1 STEP 1 UNTIL LAMMAX DO                                            SC   81   8511
READ(READER,/,FOR J + 0 STEP 1 UNTIL NT DO KAPPA[N,J] )[EXIT] ;           SC   81   8710
READ(READER,/,BKT,EKT,DKT )[EXIT] ;                                       SC   81  10A10
NKT +(EKT-BKT)/DKT  ;                                                     SC   81  11713
FOR J +2 STEP 1 UNTIL LAMMAX DO DLAMBDA[J]+LAM[J]-LAM[J-1] ;              SC   81  11912
DLAMBDA[1]+ DLAMBDA[2]  ;                                                 SC   81  12610
    BEGIN                                                                 SC   81  12712
        REAL FRI,,PHT,PHI,TAN2PHI,TANPHI,SINPHI,COSPHI,COSALPH,SINALPH,   SC   81  12712
                                                   START OF SEGMENT **********    9
```

```
        LENGTH,NOS;                                                  SC  91  010
    INTEGER NR,NPHI ;                                                SC  91  010
NR← 0 ;                                                              SC  91  010
FOR  FRI ← .1, .2, .35, .5, .6, .7, .8, .85, .9, .95, 1  DO          SC  91  013
    BEGIN                                                            SC  91 2311
    NR ← NR +1 ; NPHI← 0  ;                                          SC  91 2311
    LPHI ← IF FRI ≠ 1 THEN DPHI×.5 ELSE 1.57079632AA ←DPHI×.5  ;     SC  91 2511
    FOR PHI←LPHI STEP DPHI UNTIL NPHI DO                             SC  91 2912
    BEGIN                                                            SC  91 4210
    NPHI←NPHI+1 ;                                                    SC  91 4210
    TAN2PHI←(TANPHI←(SINPHI←SIN(PHI))/COSPHI←COS(PHI))*2  ;          SC  91 4311
    COSALPH←(FRI×TAN2PHI−SQRT(1+TAN2PHI×(1−FRI*2)))/(1+TAN2PHI)  ;   SC  91 4712
    SINALPH←SQRT(1−COSALPH*2) ;                                      SC  91 5213
    IF ABS(SINALPH/(COSALPH−FRI)−TANPHI) >.0000001 THEN              SC  91 5510
        BEGIN                                                        SC  91 5712
    COSALPH←(FRI×TAN2PHI+SQRT(1+TAN2PHI×(1−FRI*2)))/(1+TAN2PHI)  ;   SC  91 5810
    SINALPH←SQRT(1−COSALPH*2) ;                                      SC  91 6311
        END ;  LENGTH ←SINALPH×R/SINPHI ;                            SC  91 6512
    NOS←ENTIER(LENGTH/APPROXDS) +1 ;                                 SC  91 6711
    NS[NR,NPHI]←LENGTH−(DS[NR,NPHI]←LENGTH/NOS)/2×.8  ;              SC  91 7010
    C[NR,NPHI]←COSPHI  ;                                             SC  91 7513
    END ; MAX[NR]←NPHI ; END; END ;                                  SC  91 7713
                                                9 IS   87 LONG, NEXT SEG    8


EXACT ;                                                              SC  81 12810
FOR N←0 STEP 1 UNTIL 50 DO                                           SC  81 12810
    BEGIN                                                            SC  81 12910
    RT[N]←N×R/50 ;                                                   SC  81 12910
    TR[N]←ILAG(RR[N+1],ST,NAT,  RXT,DRT) ;                           SC  81 13111
    END ;                                                            SC  81 13511
TR[51]←TR[50]  ;                                                     SC  81 13712
N←0 ;                                                                SC  81 13910
    FOR  X←0,0.1, .2, .35, .5, .6, .7, .8, .85, .9, .95, 1  DO       SC  81 13913
    BEGIN                                                            SC  81 14411
    RI[N]←X×R ;                                                      SC  81 14411
    TRI[N]← ULAG(X×R,RT,TR,50) ;                                     SC  81 14610
    N←N+1  ;                                                         SC  81 17010
    END  ;                                                           SC  81 17111
FOR N ←1 STEP 1 UNTIL 11 DO                                          SC  81 18210
    BEGIN                                                            SC  81 18310
    A←RI[N]  ;                                                       SC  81 18310
    SUMF ← 0;                                                        SC  81 18410
    FOR  PHI ← 1 STEP 1 UNTIL MAX[N] DO                              SC  81 18413
        BEGIN                                                        SC  81 18813
        SUM←0 ;                                                      SC  81 18813
X←NS[N,PHI]  ; W←C[N,PHI] ; D←DS[N,PHI] ;                            SC  81 18912
        FOR J ←1 STEP 1 UNTIL LAMMAX DO FXPARG[J]←0 ;                SC  81 19413
```

```
        VM + 0 ;                                                        SC   8: 19912
        FOR S+X/2 STEP X UNTIL 0 DO                                     SC   8: 20011
            BEGIN                                                       SC   8: 20512
            RSMXY +SQRT((A      )+2 + 2XAXSX R              +S+2 ) ;    SC   8: 20512
            TM+ LAG(RSMXY,0,R/50,.R,51) ;                               SC   8: 21011
            IRM + 1.44022/TM  ;                                         SC   8: 21312
            ZM+U  ;                                                     SC   8: 21413
            FOR J + Z STEP 1 UNTIL LAMMAX DO                            SC   8: 21512
                BEGIN                                                   SC   8: 21810
                LAMBDA +LAM[J]  ;                                       SC   8: 21810
                KLM + LAG(TM,BT,DT,KAPP[(J,=1,NT ) ;                    SC   8: 21910
                IBR + 1.19250-12/(LAMBDA+5 X(EXP(IRM/LAMBDA)-1)) ;      SC   8: 222:0
                TEMP + KLMXX/2+EXPARG[J]  ;                             SC   8: 22613
                EXPARG[J]+   XXKLN + EXPARG[J] ;                        SC   8: 22911
                IF TEMP < 30  THEN                                      SC   8: 23:13
                BEGIN                                                   SC   8: 23212
                YMT+ KLMXIRRXLAG(TEMP,0,,1,G,300) ;                     SC   8:  3310
                ZM +       YMTX DLAMBDA[J] +ZM  ;                       SC   8: 23613
                END  TEMP30 ;                                           SC   8: 23813
            END OF LAMBDA LOOP  ;                                       SC   8: 23813
            VM + ZM + VM  ;                                             SC   8: 24110
        END OF S LOOP  ;                                                SC   8: 24211
        SUM +       VMXX + SUM  ;                                       SC   8: 24510


        SUMI+ SUMXR + SURF  ;                                           SC   8: 24613
    END OF  PHI  LOOP  ;                                                SC   8: 24812
   FRX[N]+ SUMFXAXDPHI ;                                                SC   8: 24910
END OF N LOOP ;                                                         SC   8: 25111
 IF  Z=1   THEN  APPF + FALSE  ELSE  APPF + TRUE  ;                     SC   8: 25312
 IF  APPF   THEN   BEGIN                                                SC   8: 25613
IF COUNT >1 THEN GO APPROX ;                                            SC   8: 25712
BEGIN                                                                   SC   8: 25813
COMMENT FORMING TABLES OF PP(T),KR(T),KP(T) FOR APPROX SOLUTIONS  ;     SC   8: 25813
REAL KRINT,KPINT;                                                       SC   8: 25813
                                                        START OF SEGMENT **********   10
ARRAY PBP[0:50,-1:36] ;                                                 SC  10:   010
FOR J+ 1 STEP 1 UNTIL Z DO                                              SC  10:   210
    BEGIN                                                               SC  10:   310
    LAMBDA+LAM[J];                                                      SC  10:   310
    IRM+ 1.44022/LAMBDA ;                                               SC  10:   410
    TEMP+LAMBDA+5  ;                                                    SC  10:   511
    I+ -1 ;                                                             SC  10:   712
    FOR X +HI STEP DT UNTIL ET DO                                       SC  10:   812
    PBR[J,I+I+1]+1.19250-12/(TEMPX(EXP(IRM/X)-1)) ;                     SC  10:  1110
    PBR[J,-1]+2XPBR[J,0]-PBR[J,1] ;                                     SC  10:  2011
    PBR[J,NT+1]+2XPBR[J,NT]-PBB(J,NT-1] ;                               SC  10:  2710
    END OF PBR TABULATION ;                                             SC  10:  3412
```

```
FOR I +0 STEP 1 UNTIL NT DO                                   SC  101  3613
    BEGIN                                                     SC  101  3910
    RB[I]+0 ;                                                 SC  101  3910
    FOR J+ 1 STEP 1 UNTIL 2 DO                                SC  101  4011
    BB[I]+        PBR(J,I]*DLAMBDA[J] +RB[I]  ;               SC  101  4110
    END OF RB TABULATION ;                                    SC  101  4712
    RB[NT+1]+ 2*RB[NT]-RB[NT-1] ;                             SC  101  4913
FOR I + 0 STEP 1 UNTIL NT DO                                  SC  101  5312
    BEGIN                                                     SC  101  5510
    KRINT+KPINT+ 0  ;                                         SC  101  5510
    FOR J + 1 STEP 1 UNTIL 2 DO                               SC  101  5611
        BEGIN                                                 SC  101  5710
        KRINT+KRINT+(PBB(J,I+1]-PBR[J,I-1])/(2*DT)*DLAMBDA(J];   SC  101  5710
        TEMP+ IF A + KAPPA[J,I]#0 THEN A ELSE P-30  ;         SC  101  6313
        KPINT + KPINT + PBR[J,I]*TEMP*DLAMBDA[J] ;            SC  101  6910
        END OF J LOOP ;                                       SC  101  7310
    IF I =0  THEN KR[0] +(RB[1]-BB[0])/DT/KRINT ELSE          SC  101  7511
    KR[I]+(BB[I+1]-BB[I-1])/(2*DT)/KRINT  ;                   SC  101  7913
    KP[I]+KPINT/BB[I] ;                                       SC  101  8613
    END OF I LOOP ;                                           SC  101  8813
COMMENT BB[T],KP[T],KR[.] TABLES NOW FORMED ;                 SC  101  9110
LITTLEB + 1 ;                                                 SC  101  9110
END ;                                                         SC  101  9113


                                        10 IS    95 LONG, NEXT SEG    8
APPROX :                                                      SC    8: 26010
BEGIN COMMENT APPROX SOLUTION ;                               SC    8: 26010
ARRAY KA,KA2,TM[0:200]  ;                                     SC    8: 26010
                                        START OF SEGMENT **********   11
FOR N +1 STEP 1 UNTIL 11 DO                                   SC  111   211
    BEGIN                                                     SC  111   310
    A+R[N]  ;                                                 SC  111   310
    SUMF + 0 ;                                                SC  111   410
    FOR PHI+ 1 STEP 1 UNTIL MAX[N] DO                         SC  111   413
        BEGIN                                                 SC  111   813
        SUM+ 0 ;                                              SC  111   813
X+DS[N,PHI]  ; W+C[N,PHI] ; D+HS[N,PHI] ;                     SC  111   912
        VM+ 0 ;                                               SC  111  1413
        TAUP2 + 0;                                            SC  111  1512
        TAUR2 + 0;                                            SC  111  1611
        RSMXY+SQRT(A*2+2*A*X*W*(S+D+.15*X)+S*2 )  ;           SC  111  1710
        TEMP+LAG(RSMXY ,0,R/50,TR,51) ;                       SC  111  2311
        KP2+ LAG(TEMP,HT,DT,KP,NT) ;                          SC  111  2612
        KR2+ LAG(TEMP,HT,DT,KR,NT) ;                          SC  111  2911
        TAUP + KP2*X/2 ;                                      SC  111  3210
        TAUR + KR2*X/2 ;                                      SC  111  3313
        COUNTS +ENTIER((S+.25*X)/APPROXDS)+2 ;                SC  111  3512
```

```
K←.A×X ;                                                          SC 111 3931
        FOR S← U        -.1×X  STEP -X UNTIL X    DO               SC 111 4012
            BEGIN                                                  SC 111 4611
            COUNTS ← COUNTS - 1 ;                                  SC 111 4611
            RSWAY ←SQRT(A↑2 +2×S×A×B +S↑2) ;                       SC 111 4712
            TEMP←TM[COUNTS]+LAG(RSWAY,0,R/50,TR,51) ;              SC 111 5211
            KPT←LAG(TEMP,RT,DT,KP,NT) ;                            SC 111 5612
            KRT←LAG(TEMP,RT,DT,KR,NT) ;                            SC 111 5911
            TAUP2←      X×KPT + TAUP2  ;                           SC 111 6210
            TAUR2←      A×KRT + TAUR2  ;                           SC 111 6313
            KA[COUNTS]←LITTLER/(TEMP←LITTLER +TAUP)×(LITTLER+TAUR)/  SC 111 6512
                         TEMP×KPT + TAUP/TEMP×KRT ;                SC 111 6613
            TEMP←LAG(SQRT( A↑2+2×A×R×(TEMP+S-X/2)+ TEMP↑2),0,R/50,TR,51)  SC 111 7113
            ;                                                      SC 111 7912
            KP2← LAG(TEMP,RT,DT,KP,NT) ;                           SC 111 8012
            KR2← LAG(TEMP,RT,DT,KR,NT) ;                           SC 111 8311
            TAUP←KP2×X+TAUP ;                                      SC 111 8610
            TAUR←KR2×A+TAUR ;                                      SC 111 8713
            KA2[COUNTS]←LITTLER/(TEMP←LITTLER+TAUP2 )×(LITTLER+TAUR2)/  SC 111 8912
                         TEMP×KR2 + TAUP2 /TEMP×KR2  ;             SC 111 9213
        END OF PRE S LOOP ;                                        SC 111 9513
        TEMP←LAG(SQRT(A↑2+2×A×R×(S+A/4)+S↑2),0,R/50,TR,51)  ;      SC 111 10210
        KPT ←LAG(TEMP,RT,DT,KP,NT) ;                               SC 111 11011


        KRT ←LAG(TEMP,RT,DT,KR,NT) ;                               SC 111 11310
        TAUP←(KPT+KP2)/2×A/A ;                                     SC 111 11513
        TAUR←(KRT+KR2)/2×X/A ;                                     SC 111 11812
        KA2[1]←(LITTLER/(TEMP←LITTLER+TAUP)×(LITTLER+TAUR)/TEMP×KPT SC 111 12011
               + TAUP/TEMP×KRT)/2 ;                                SC 111 12510
        TAUA ←0 ;                                                  SC 111 12810
        COUNTS← 0 ;                                                SC 111 12813
        FOR S← A/2 STEP X UNTIL 0          DO                      SC 111 12912
            BEGIN                                                  SC 111 13413
            COUNTS←1+COUNTS  ;                                     SC 111 13613
            RSWAY← SQRT(A×2+2×A×B×S+S×2)  ;                        SC 111 13610
            KLM ← KA[COUNTS] ;                                     SC 111 14013
            BRR ← LAG(TM[COUNTS],BT,DT,BR,NT) ;                    SC 111 14113
            TEMP ←TAUA←     KA2[COUNTS]×A + TAUA  ;                SC 111 14613
            IF TEMP >30 THEN ZM←0 ELSE ZM←KLM×BRR×LAG(TEMP,0,.1,G,300) ;  SC 111 14711
            VM← ZM + VM ;                                          SC 111 15212
        END OF S LOOP  ;                                           SC 111 15413
        SUM ←       VM×X +SUM  ;                                   SC 111 15710
        SUMF←        SUM×R +SUMF  ;                                SC 111 15813
    END OF PM1 LOOP ;                                              SC 111 16012
  FRX[N]←       SUMF×A×DPM1  + FRX[N)   ;                          SC 111 16110
END OF N1 LOOP ;                                                   SC 111 16610
END OF APPROX FLUX  ;                                              SC 111 16611
```

```
    END  OF  APPF  ;                                                    11 IS  270 LONG, NEXT SEG    8
  FRX[0]←FR[1]←0 ;                                                                 SC   8: 26110
  FOR J← 2 STEP 1 UNTIL 9[ DO                                                      SC   8: 26110
  FR[J]←ULAS(NT]J-1],R],FRX,11) ;                                                  SC   8: 24311
  COUNT ← 10 ;                                                                     SC   8: 24A10
  EXIT 1 ;                                                                         SC   8: 27012
  IF COUNT # 10 THEN                                                               SC   8: 27111
  WRITE(PRINTER,< "DATA CARDS FOR FLUX PROCEDURE ARE INCOMPLETE "> ) ;              SC   8: 27210
                                                                                   SC   8: 27213
  END OF FLUX  ;                                                       12 IS   11 LONG, NEXT SEG    8
                                                                                   SC   8: 27611
  PROCEDURE  DELSQ (N,SC)    ;                                         P IS  296 LONG, NEXT SEG    2
    VALUE  N ;   INTEGER  N  ;                                                     SC   2: 2610
    ARRAY  SC[0] ;                                                                 SC   2: 2610
  BEGIN                                                                            SC   2: 2610
    SC[1] ← A←(S[2]-S[1])/(DR←2)   ;                                               SC   2: 2610
    FOR  I←2   SL   N   DO                                                         SC   2: 2610
      SC[I]←(S[I+1]-S[I-1])×0.5/(DR×R[I]) +(S[I+1]+S[I-1]-S[I]×2)/(DR←2) ;         SC   2: 3013
  END  OF  DELSQ  ;                                                                SC   2: 3210
  PROCEDURE   TRIDAG (N, A,B,C,D )  ;                                              SC   2: 4013
  ARRAY A,B,C,D[0]  ;    INTEGER  N   ;                                           SC   2: 4610
  COMMENT  PROCEDURE FOR INVERTING TRIDIAGONAL MATRIX OF N×N    ;                  SC   2: 4610
                                                                                   SC   2: 4610
    BEGIN    REAL  Z;    INTEGER  J  ;                                           SC   2: 4610
                                                                         START OF SEGMENT ••••••••••   13
    D[1] ← D[1]/B[1] ;                                                           SC  13:  010
    Z← B[1] ;                                                                    SC  13:  211
    FOR  J← 2  SL  N  DO                                                         SC  13:  311
      BEGIN   B[J-1] ← C[J-1]/Z  ;                                               SC  13:  410
      Z ←B[J] ← A[J-1] × B[J-1] ;                                                SC  13:  710
      D[J] ← (D[J]- A[J-1]× D[J-1])/Z  ;                                         SC  13: 1012
      END ;                                                                      SC  13: 1510
    FOR J←[ SL   N-1  DO                                                         SC  13: 1711
      D[N-J] ← D[N-J] -B[N-J]× D[N-J+1]   ;                                      SC  13: 2112
    END  TRIDAG   ;                                                              SC  13: 2712
                                                                         13 IS   30 LONG, NEXT SEG    2
  PROCEDURE   DVGVT  (N,SM, F, DGV )     ;                                     SC   2: 4610
    ARRAY  SM, F, DGV[0]   ;   INTEGER   N  ;                                    SC   2: 4610
  COMMENT  PROCEDURE FOR EVALUATING THE DIVERGENCE OF FLUX  ;                    SC   2: 4610
  BEGIN    REAL  P,ZJ    INTEGER I, J  ;                                       SC   2: 4610
                                                                         START OF SEGMENT ••••••••••   14
  P← F[2]×2/DR -×(S[2]-S[1])/(DR←2) ;  P←ABS(P)/E← SQRT(P/SIGMA[1])  ;            SC  1A:  010
    DVGF[1] ← F[2]×2/DR  ;                                                       SC  1A:  810
      SE0][] ← SIGMA][] ×E←2  ;                                                  SC  1A: 1012
    FOR  I←2  SL  N  DO  BEGIN                                                   SC  1A: 1310
      DVGF[I] ← (F[I+1]-F[I-1])/(2×DR) + F[I]/R[I]   ;                           SC  1A: 1410
```

```
SEG[I] ← SIGMA[I] × E+2   ;                                          SC  14:  1013
DGV[I] ←  SEG[I] - DVGF[I]   ;                                       SC  14:  7211
END  I?  ;                                                           SC  14:  7412
DGV[I] ← SIGMA[I] × E+2 - F[2]×2/DR   ;                              SC  14:  7613
END  DVGVT     ;                                                     SC  ?1:  3110
                                                  1A IS   ?A LONG, NEXT SEG    2
COMMENT  XCHANGE (VERSION OF 4/1/6?);                       00000000 SL   21  A610
                                                            99999999 SC   21  A011
COMMENT  PRELIMINARY CALCULATIONS   ;                                SC   21  A011
 TIME1(PRINTER );                                                    SC   21  A011
 BETA ← 1.0 ;  M ← 90  ;                                             SC   21  A210
READ(READER, /, RB, N )  ;                                           SC   21  63.2
COUNT←0 ;                                                            SC   21  7513
READ(READER, /, DT,NT )  ;                                           SC   21  7612
  NN ←   N + 1  ;                                                    SC   21  8713
  DR ← RB/N     ;                                                    SC   21  8910
 FOR I ← 1  SL    NN   DO   R[I] ← (I-1)×DR    ;                     SC   21  9011
  RHO ← BETA×DT /(DR×2) ;                                            SC   21  9512
  LDA ← BETA×DT /(2×DR) ;                                            SC   21  9713
  R[5I] ← 0; R[5I]← RB  ;                                            SC   21 10010
  A[I] ← LDA/DR - RHO  ;                                             SC   21 10212
  C[I] ← - A×RHO  ;                                                  SC   21 10413
  B[I] ← 1+ A×RHO  ;                                                 SC   21 10613


 FOR I←2  SL    N   DO  BEGIN                                        SC   21 10910
   A[I]← (LDA/R[I+1] -RHO ) ;                                        SC   21 11010
   C[I] ← -(RHO +LDA/R[I])  ;                                        SC   21 11310
 END I   ;                                                           SC   21 11513
READ (READER,// FOR  I←1  SL  51  DO  T[I] ) ;                       SC   21 11810
READ(READER ,// FOR I← 0  SL  N     DO   (ST[I], SMY[I] ) )   ;      SC   21 13013
K← 0  ;  THE[0] ←0  ;                                                SC   21 14513
FOR  I←1  SL    NN    DO  S[I] ←  LAG(T[I], 2000, 200, ST, M)  ;     SC   21 14713
COMMENT  MAIN PROGRAM AND NEW TIME SOLUTIONS START HERE    ;         SC   21 15413
START ;                                                              SC   21 15413
  WRITE(PRINTER, FMT;, FOR  I←1  SL  NN  DO  S[I] )  ;               SC   21 15510
FOR  I←1   SL    NN    DO  SIGMA[I]← ULAG(S[I],ST, SMY,  M   )    ;  SC   21 16811
IF  K # 0  THEN                                                      SC   21 17510
FOR  I←1  SL  NN  DO  T[I] ← ILAG(S[I], ST, M, 2000, 200 )   ;       SC   21 17513
 WRITE(PRINTER[PAGE] );                                              SC   21 18213
 WRITE(PRINTER, <X3, "AT TIME=", X12.5, X3,"SECONDS", //>, THE[K])  ; SC   21 18512
                                                  15 IS   12 LONG, NEXT SEG    2
 FLUX (S, F, RB)  ;                                                  SC   21 19611
IF   COUNT # 10  THEN  GO  EXIT  ;                                   SC   21 19812
 DVGVT (N  , SIGMA, F, DGV )  ;                                      SC   21 19913
  DELSW (N, SC)   ;                                                  SC   21 20213
FOR  I←1  SL   N  DO  SS[I] ← SC[I] + SEG[I] - DVGF[I]  ;            SC   21 20411
WRITE(PRINT/R,  H01 )  ;                                             SC   21 21011
```

```
    WRITE(PRINTER, FMT1, FOR I←1 SL NN DO I[I],S[I],F[I], T[I],                    SC   21 21311
    SIGMA[I],SC[I], DVGF[I], SEC[I], SS[I] ) )  ;                                  SC   21 22610
    WRITE(PRINTER[DBL] ] ;                                                         SC   21 23811
    WRITE (PRINTER, <X3, "E =", F10.4,//>, F )  ;                                  SC   21 24110
                                                                 16 IS    8 LONG, NEXT SEG    2
    AI ←0.0  ;                                                                     SC   21 24811
    FOR I←1  SL  NN DO   BEGIN                                                     SC   21 24910
   IFC← IF  I=1  OR  I=NN  THEN  1  ELSE  IF  (I-1)  MOD  2 = 0  THEN  2           SC   21 25010
     ELSE  4   ;                                                                   SC   21 25413
    AI ← AI + 2×3.1415926×E×R[I]×SIGMA[I]×IFC       ;                              SC   21 25613
    END  INT ;                                                                     SC   21 26110
    AI ← AI×DR/3     ;                                                             SC   21 26311
     WRITE(PRINTER, <//,X3,"ARC CURRENT I=", E12.5,//>, AI)  ;                     SC   21 26510
                                                                 17 IS   12 LONG, NEXT SEG    2
  TIMEIT(PRINTER) ;                                                                SC   21 27311
    IF  K= NT  THEN  WRITE(PUNCH, <5(E12.5,", "  )>, FOR  I←1  SL  NN   DO         SC   21 27411
                                                                 18 IS    7 LONG, NEXT SEG    2
       T[I] )  ;                                                                   SC   21 28111
    IF  K ≥ NT THEN  GO  TO  EXIT  ;                                               SC   21 28811
    TN[K+1]← TN[K] + DT  ;          K← K+1   ;                                     SC   21 28912
    FOR I←1  SL  N  DO              D[I] ←   T[I] + DGV[I]×BETA×DT     ;           SC   21 29311
    B[I] ←  1 + A×RHO  ;                                                           SC   21 29912
   FOR I←2  SL  N  DO  B[I] ← 1+ 2×RHO  ;                                          SC   21 30113
    TRIDAG (N, A, B,C, D)    ;                                                     SC   21 30712


   EXCHANGE( S,D )   ;                                                             SC   21 31111
   GO  TO  START       ;                                                           SC   21 313.3
  EXIT:                                                                            SC   21 31411
   TIMEIT (PRINTER );                                                              SC   21 31510
  END.                                                                             SC   21 31610
                                                                 2 IS  319 LONG, NEXT SEG    1
 COS           IS SEGMENT NUMBER 0019, PRT ADDRESS IS 0155
 EXP                          0020              0160
 SIN                          0021              0154
 SQRT                         0022              0156
 OUTPUT(W)                    0023              0102
 BLOCK CONTROL                0024              0005
 INPUT(W)                     0025              0144
 GO TO SOLVER                 0026              0146
 ALGOL WRITE                  0027              0014
 ALGOL READ                   0028              0015
 ALGOL SELECT                 0029              0016
NUMBER OF ERRORS DETECTED =    0                  LAST CARD WITH ERROR HAS SEQ #
PRT SIZE = 156; TOTAL PGM SEGM SIZE =  1404 WORDS; DISK SIZE =  80 SEGS; NO. PGM. SEGS =  30
ESTIMATED CORE STORAGE REQUIREMENT =  6630 WORDS.
16159142 WEDNESDAY, JUNE 7, 1967    PROCESSOR TIME = 31.60 SECONDS    I/O TIME = 31.62 SECONDS
```

APPENDIX F

Analysis of Xenon Discharges

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I. INTRODUCTION

Calculations have been performed deriving temperature profiles of discharges in xenon flash tubes from given material functions for xenon, at a specified experimental value of current and electric field strength. The calculations include the effects of conduction, radiation, and self absorption of radiation. Comparisons are made of three different methods of doing these calculations. Results of these calculations indicate that for typical values of electric field strength and current the temperature profiles are radiation dominated if the pressure is equal to or higher than four atmospheres, the profiles are relatively flat, the influence of radiation at wavelengths less than 1000Å is negligible, and the effect of self absorption in the visible continuum is of only secondary importance in determining the central temperature.

An analysis has been made of the time dependence of the experimental data of electric field strength, current and radiation. The radiation measurements suggest that the xenon discharge should be treated as a time dependent problem rather than a wall stabilized, steady state arc, which is the basis of the present calculations.

II. TEMPERATURE PROFILE CALCULATIONS

Calculations of the temperature profile for a wall stabilized steady state arc for a given electric field strength, current and gas pressure have been made using (1) the Eddington Approximation, (2) a pseudo time dependent equation and an exact radiation flux calculation and (3) a pseudo time dependent equation and an exact radiation intensity calculation. It is considered that method (3) is the least expensive. However, for comparison of calculated values of central temperature and arc radius with experiment, a simple constant temperature model is adequate.

The input material functions for the calculations are those supplied by C. H. Church. The spectral absorptivities are an estimate of the continuum and neglect line radiation. Thermal and electrical conductivities are calculated using a program of De Voto. The effects of radiation were determined by dividing the spectrum into 20 equal frequency bands extending to 5×10^{16} Hz(600Å).

1. Method using Eddington Approximation

   This method is outlined in reference (1). The following equations are solved numerically.

$$\nabla.(\vec{F}_c + \vec{F}_R) = \sigma E^2 \tag{1}$$

$$\vec{F}_C = -k\nabla T \tag{2}$$

$$\vec{F}_R = \int \vec{F}_{R\nu} d\nu \tag{3}$$

$$\nabla.\vec{F}_{R\nu} = 4\pi\ (\varepsilon_\nu - J_\nu K_\nu) \tag{4}$$

$$\vec{F}_{R\nu} = -\frac{4\pi}{3K_\nu}\ \nabla J_\nu \tag{5}$$

The nomenclature is given in Table I.

Equation (5) is the only inexact equation and is known in astrophysics as the Eddington approximation. The equation is in effect a diffusion approximation for the radiation flux and is equal to a constant multiplied by the gradient of the radiation energy density, which is proportional to ∇J_ν. An iterative procedure is used to satisfy the boundary conditions which are as follows

at $r = 0$ $\quad F_{R\nu} = 0$ $\quad$ and $F_T = 0$

at $r = R$ $\quad T = T_W$ $\quad$ and $J_\nu = \frac{2}{\pi^2} F_{R\nu}$.

Table I

Nomenclature

$\vec{F}_C$	Conduction Flux Density	(watts cm^{-2})
$\vec{F}_R$	Radiation Flux Density	(watts cm^{-2})
k	Thermal Conductivity	(watts $cm^{-1}{}^\circ K^{-1}$)
σ	Electrical Conductivity	(mho cm^{-1})
K_ν	Spectral Absorbtivity	(cm^{-1})
ϵ_ν	Spectral Emission Coefficient	(watts $cm^{-3}ster^{-1}sec$)
$\vec{F}_{R\nu}$	Radiation Flux Density per unit Frequency	(watts $cm^{-2}sec$)
J_ν	Radiation Intensity per unit Frequency	(watts $cm^{-2}ster^{-1}sec$)
T	Temperature	(°K)
E	Electric Field Strength	(volt cm^{-1})
I	Electric Current	(amps)
r	Radius	(cm)
T_w	Wall Temperature	(°K)
C_p	Specific Heat at Constant Pressure	(Joules $gm^{-1}{}^\circ K^{-1}$)
ρ	Density	(gm cm^{-3})
ϵ	Integrated Emission Coefficient	(watts $cm^{-3}ster^{-1}$)
t	Time	(sec)
B_ν	Planck Function	(watts $cm^{-2}ster^{-1}sec$)
p	Pressure	(Atmospheres)

Input values are the material functions k, σ, K_ν and ϵ_ν (which are functions of temperature), and the experimental values of I and E. R is determined from

$$2\pi R(F_c + F_R)_{r=R} = IE \qquad (6)$$

The solution of these equations giving T, F_R and F_C as a function of radius for E = 29 volt/cm and I = 1140 amps at a pressure of 11 atmospheres is shown in Fig. 1.

2. Method using a pseudo time dependent equation and an exact radiation flux calculation

This method has been suggested by B. Swanson.

Rather than iterate to satisfy split boundary conditions as in the former method, an assumed initial temperature profile is modified using the time dependent equation to obtain the steady state solution.

The time dependent equation, neglecting effects of mass flow is given by equation (7)

$$C_p \rho \frac{\partial T}{\partial t} = \sigma E^2 - \nabla.\vec{F}_C - \nabla.\vec{F}_R \qquad (7)$$

As we are only interested in obtaining the steady state solution, $C_p\rho$ is made equal to 1, a constant. $\vec{F}_C$ is obtained using equation (2) and $\vec{F}_R$ is obtained exactly using the integration procedure of Swanson.[2] A number of difficulties associated with this method are overcome as described below.

(1) The numerical solution of this equation is unstable for large step sizes in time. This instability is described by Richtmyer[3] and in the present method of solving the equation, the size of the time step for stability has been empirically found to closely follow the requirement cited by Richtmyer that

$$\Delta t < \frac{(\Delta r)^2}{2F} \quad \text{where } F = k/\rho C_p \ . \tag{8}$$

Generally the small step size requirement makes computing times prohibitively large. However in radiation dominated arcs, the temperature of most of the arc is controlled by the terms $\sigma E^2 - 7.\vec{F}_R$ of equation (7) and not by ∇F_c which causes the instability. By initially dividing the term $\nabla.\vec{F}_c$ by a factor of the order of 30 and increasing the step size by the same factor the rate of convergence to the final profile is greatly increased. The multiplying factor is then removed to determine the outer small region of the profile, which is controlled by conduction. In this latter stage of the calculation it is only necessary to recalculate $\vec{F}_R$, which is the most time consuming part of the calculation, at say every twentieth time step, for $\vec{F}_R$ is determined primarily by

the temperature of the inner region of the arc. With this simplification any initial temperature profile can be made to rapidly converge to the final solution.

(2) In the present problem, current and electric field strength are input values and the radius and the temperature profile are the output. After each time step the radius is recalculated using equation (9), where the temperature profile is regarded as a function of r/R

$$R^2 = I[2\pi E \int_0^1 x\sigma dx]^{-1} \qquad (9)$$

where x = r/R.

In this way the correct current is maintained as the temperature profile is varied.

(3) It is found that the temperature profile can vary monotonically and very slowly in a way making it difficult to determine the error from the true steady state solution. To test for convergence, after calculating each new temperature profile, equations (1) and (2) are solved to obtain $\vec{F}_R$ as a function of r. If the temperature profile is correct, the values of $\vec{F}_R$ will agree with the values of $\vec{F}_R$ obtained from the spectral absorbtivities using the Swanson exact integration procedure.

In the numerical results presented using this method the two values of $\vec{F}_R$ agree to 1% in each case. The method was used for the conditions of Fig. 1 and the temperature profile is shown as the broken curve. The small difference in the profiles near the outer wall is considered to be due to an insufficiently small step size in method 2 and not due to the Eddington approximation. The step size in r/R near the wall in method 2 was 0.01 whereas in the Eddington method it was 0.0001.

The method was also used for p = 4 Atmospheres with E = 29 volt cm^{-1} and I = 1140 amps giving results insignificantly different from those shown in Fig. 2, which were obtained using method 3. Fig 3 gives results obtained using method 2 showing the variation of $F_{R\nu}$ with r at two different frequencies. The radiation flux integrated from the absorption edge at $\nu = 2.9 \times 10^{15}$ to $\nu = 5 \times 10^{15}$ Hz attains a maximum of only 2% of the total radiation flux at r/R = 0.87 for the conditions of Fig. 2. The inclusion of lines in this region of the spectrum will only decrease the radiation flux as, from the Eddington Approximation, which is equation (5), K_ν is increased in the region of lines and $J_\nu \sim B_\nu$ (see Fig. 4). Consequently it is concluded that, except for very high powers where the central temperature is greater than 14000°K, the effect of radiation for wavelengths less than 1000A can generally be neglected in the present calculations.

3. Method using a pseudo time dependent equation and exact radiation intensity calculations

For the conditions of the present problem it is of considerable advantage to express equation (7) in the form

$$C_p \rho \frac{\partial T}{\partial t} = \sigma E^2 - \nabla.\vec{F}_c - 4\pi(\epsilon - \int J_\nu K_\nu d\nu) \qquad (10)$$

where use is made of the continuity equation for radiation, equation (4). From Kirchoff's Law $\epsilon = \int B_\nu K_\nu d\nu$ and ϵ is simply a function of temperature. J_ν can be obtained exactly from a modification of the Swanson integration procedure used to obtain $\vec{F}_R$.

The advantages of this modification to method 2 are

a. The increment in temperature does not depend on the gradient of a computed quantity. In method 2 to determine $\nabla.F_R$, F_R needs to be calculated to high accuracy and at many radial steps.

b. For typical experimental conditions in xenon, $\int J_\nu K_\nu d\nu$ is small compared with ϵ, provided that ultraviolet radiation can be neglected. Then the integral need only be calculated at say every 100th step, instead of after every 20th step, as outlined in the latter part of Section

II 2 (1). In fact if the integral in the visible range of the spectrum is set at zero, the central temperature is decreased by only 200°K for Fig. 1 and 300°K for Fig. 2.

Instead of having E and I as the input, as in method 2, E and R are treated as the input and the value of I is calculated as output. The difficulty outlined in II 2 (2) is thus removed and the stability of the numerical solution is also improved.

The profile obtained using this method, with E = 29 and R = 0.1 as input at a pressure of 4 Atmospheres is shown in Fig. 2. Fig. 4 gives J_ν as a function of frequency at two radial points.

4. Constant temperature model

In any comparison of theoretically derived temperature profiles with experiment one of the principal interests is to compare, for any value of I and E, the theoretical central temperature and radius with experimental observations. An assessment can then be made of the accuracy of the input material functions, σ and K_ν, assuming that the experimental arc is wall stabilized and in an effective steady state condition. For this purpose, for the experimental conditions considered in this paper, the central temperature and R can be computed to within 5% simply by assuming that the arc is at constant temperature, without computing the temperature profile.

For radiation dominated arcs, loss of energy by conduction at the center of the arc is negligible compared with radiation losses. Thus the input electrical energy equals the net emission of radiation energy, as expressed in equation (11), i.e.,

$$\sigma E^2 = 4\pi(\varepsilon - \int J_\nu K_\nu d\nu) \qquad (11)$$

At the center of a cylindrical plasma of radius R and uniform temperature T, J_ν can be calculated using the two radiation equations (4) and (5) again given below

$$\nabla . \vec{F}_{RV} = 4\pi(\varepsilon_\nu - J_\nu K_\nu)$$

$$\vec{F}_R = - \frac{4\pi}{3K_\nu} \nabla J_\nu$$

As ε_ν and K_ν are constant the equations can be solved analytically to give

$$J_\nu(o) = B_\nu \{1 - 1/(I_o(y) + \frac{8}{\sqrt{3}\,\pi} I_1(y))\} \qquad (12)$$

where $y = \sqrt{3}\ K_\nu R$ and I_o and I_1 are modified Bessel Functions.

In this way the integral in equation (11) can be evaluated, and the equation used to determine E for any given cylinder of radius R and temperature T. The current I is then obtained from the conductivity equation (13)

$$I/E = \pi R^2 \sigma \qquad (13)$$

Curves computed using equations (11), (12) and (13) are given in Figs. 5, 6 and 7 for pressures of 2.5, 4 and 11 atmospheres respectively. The agreement of the central temperature and radius predicted for pressures of 4 and 11 atmospheres for E = 29 and I = 1140 with the temperature profiles of Figs. 1 and 2 is within 5%.

For p = 2.5 Atmospheres, the point at E = 29 volt cm^{-1} and I = 1140 amperes appears to be just in the folded region of the curves of Fig. 5 where multiple solutions are possible. The existence of multiple solutions has been investigated but for other input material functions and for a different gas and will be reported later. For xenon at 2.5 Atmospheres, for E greater than 30 and I = 1140 the only solution that exists is for a conduction dominated arc where the central temperature is controlled by thermal conduction and not by radiation. At E = 29 volt cm^{-1} I = 1140 amperes the only solution that was found was that of a conduction dominated arc with a central temperature above 19,000°K. At these temperatures the input material functions are unknown. No detailed search was made for the existence of a solution corresponding to a radiation dominated arc for this value of E and I.

III. COMPARISON WITH EXPERIMENT

1. Steady state condition

For a tube of R = 0.63 cm the peak values of I, E and temperature that have been measured are E = 29 volt cm^{-1}, I = 1140 amps, central temperature = 11,500°K and pressure = 4.2 atmospheres.[4] As these quantities apply for a time corresponding to $\frac{\partial T}{\partial t} = 0$ it should be appropriate to compare with the steady state theoretical solution. Upper and lower limits of the possible gas pressure are 11 and 2.5 Atmospheres.

Results obtained from Fig. 6, and for similar curves at 4 Atmospheres but with different values of σ and K_ν are given in Table 2.

Table 2 (p = 4, E = 29, I = 1140)

Input		Output	
σ	K_ν	R	T
De Votto Values	Normal Continuum	0.4	13,300
De Votto Values	2 x Continuum	0.42	11,700
1/2 x De Votto	Normal Continuum	0.6	11,700
1/2 x De Votto	2 x Continuum	0.62	10,800

If lines are included in the spectral absorbtivity data, the integrated emission coefficient may be increased by a factor of two. However, as is seen from Table 2, the computed radius is still only 0.42 cm and σ would stillneed to be decreased for the arc to fill the tube.

Unfortunately measurements of the discharge radius are difficult to make. Furthermore no accurate experimental measurements of σ for xenon are known. It is seen that the theoretical predictions are in very approximate agreement with experiment, but if the discharge does indeed fill the discharge tube it would appear that the De Vott σ values of σ are too high. However an analysis of the time dependence of the experimental parameters suggests that the discharge does not fill the tube. Therefore it should not be concluded that we believe that the σ or σ data is in error.

2. Time dependence of the discharge

From the time dependence of the experimentally[4] observed values of E, I and radiation intensity at 8232Å, the curves of Fig. 8 and 9 have been prepared. In Fig. 8 it is seenthat the curves for differing discharge energies are in reasonable coincidence for the latter portion of the discharge time. However it is seen in Fig. 9 that the radiation intensity at a particular value of I varies markedly for discharges of differing input power. If the discharge were to be wall stabilized and effectively in the steady state condition, the value of E and central temperature (and thus

the radiation intensity) would be determined for any value of R and I. If the experimental measurements are correct, it appears that the arc cannot be regarded as being wall stabilized and in the steady state at times after the peak radiation intensity.

It is known that the pressure inside of the discharge tube is determined not only by the core temperature, but is controlled to a large extent by the temperature of the gas near the tube wall. It is suggested that this gas is continually heated throughout the duration of the pulse, thus increasing the pressure. The central temperature, which is determined from equation (11), is thus lower at a given I for pulses of high power because the gas pressure is higher. In this way it may be possible to explain the radiation measurements of Fig. 9. It would then be expected that the radius of the central portion of the arc does not fill the tube, and increases throughout the duration of the pulse.

Measurements of the temperature profile at peak power are consistent with the theoretical predictions that the temperature profile is very flat.

IV. CONCLUSIONS

For the experimental parameters typical for the operation of xenon flash tubes, the following generalizations can be made.

1. The temperature profiles are very flat and are radiation dominated, provided the gas pressure equals or is greater than 4 Atmospheres.

2. Except for very high powers where the central temperature is above 14,000°K, the effect of radiation of wavelengths less than 1000Å can be neglected.
3. Self absorption effects in the visible continuum generally effect the central temperature by less than 1000°K.
4. The constant temperature model in which account is taken of absorption, can be used to predict the central temperature and outer radius of wall stabilized arcs to within 10%.
5. Of the three methods used to compute temperature profiles of steady state, wall stabilized arcs from input material functions, it appears that the time deperdent method using an exact radiation intensity calculation is the most economic.
6. Experimental measurements indicate that the arc discharge is not wall stabilized and that time dependent studies are needed.

V. POSSIBLE FUTURE WORK

1. Experimental

   (1) Time dependent studies of the radiation intensity as a function of radius are needed to determine whether the radius varies with time.

   (2) Improved measurements of the pressure as a function of time.

   (3) Measurements of temperature profiles of a cascade arc in xenon. Such a measurement would enable a determination of electrical conductivity, which is a crucial input parameter in the theoretical calculation of temperature profiles.

2. Theoretical

(1) If the pressure and E were known as a function of time, a time dependent study using equation (10) could be made to predict the current and the temperature profile as a function of time. The self-absorption integral of equation (10) could be neglected giving very considerable improvement in computation time and an error of only a few hundred degrees in the central temperature. It is proposed that for a given I the temperature of the gas near the quartz walls which contain the arc, is dependent on the total power fed into the pulse, but that the temperature profile of the arc core at late times is relatively insensitive to the initial temperature profile that is assumed for the calculations. The gas pressure as a function of time could be derived from the computed temperature profiles and compared with the input pressure as a function of time.

(2) A more involved computation could be carried out solving equations (14), (15) and (16)

$$C_p \rho \left(\frac{\partial T}{\partial t} + \underline{v} \cdot \nabla T\right) - \nabla \cdot (k \nabla T) + v \frac{\partial v}{\partial t} + v\, \underline{v} \cdot \nabla v$$

$$- \sigma \vec{E}^2 - 4\pi - \frac{1}{\rho} \frac{\partial p}{\partial t} = 0 \qquad (14)$$

$$\rho \frac{\partial \underline{v}}{\partial t} + \rho\, \underline{v} \cdot \nabla \underline{v} = -\nabla p \qquad (15)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \underline{v} = 0 \qquad (16)$$

As p and ρ determine T; p, ρ, v and T can be determined as a function of time and compared with experiments.

VI. ACKNOWLEDGEMENT

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3. R. D. Richtmyer, "Difference Methods for Initial Value Problems", Interscience (1957).

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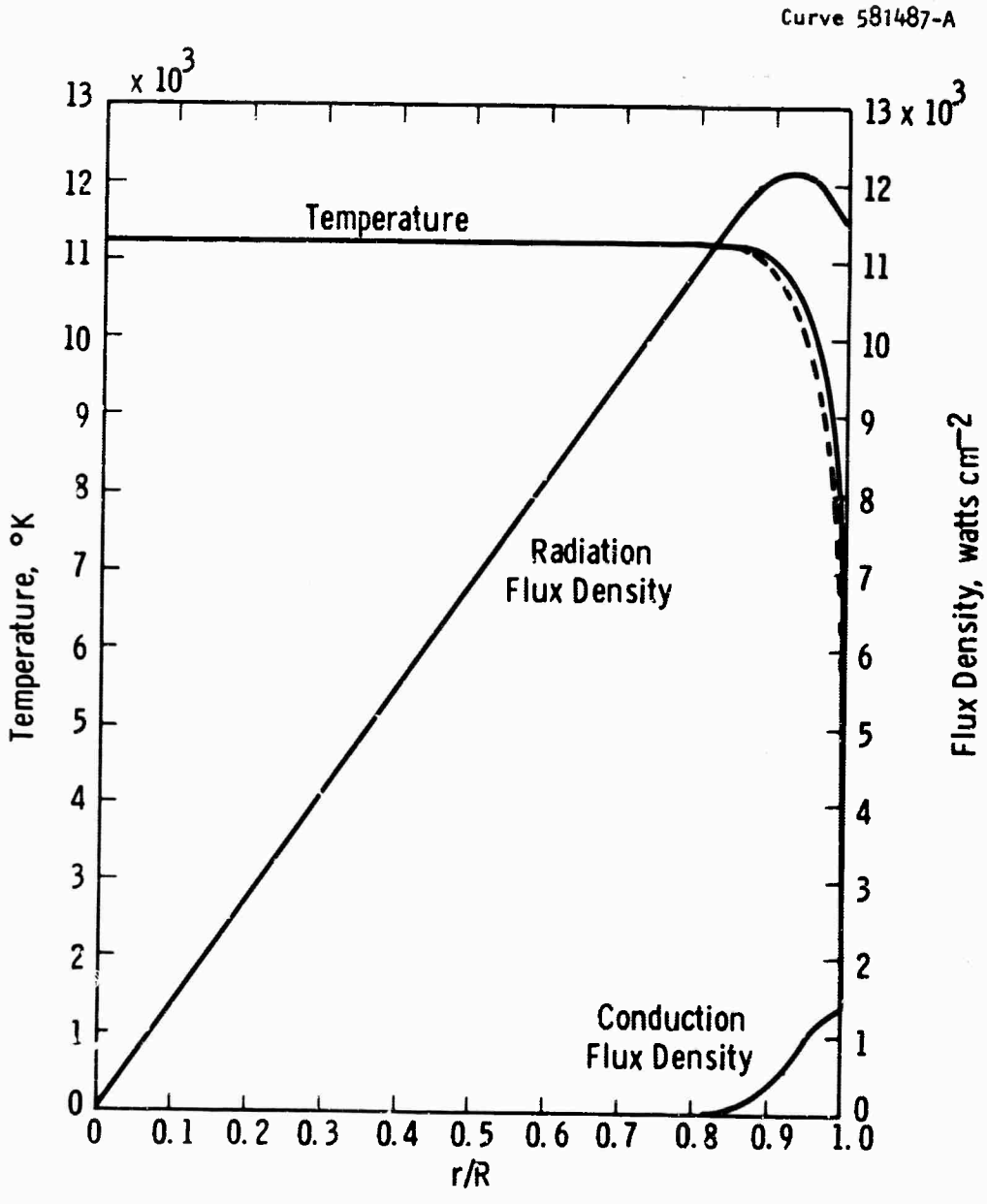

Fig. 1—Xenon arc profile

Input: p = 11 Atm, E = 29 V/cm, I = 1140 Amp, T_W = 2000°K
Output: R = 0.410 cm

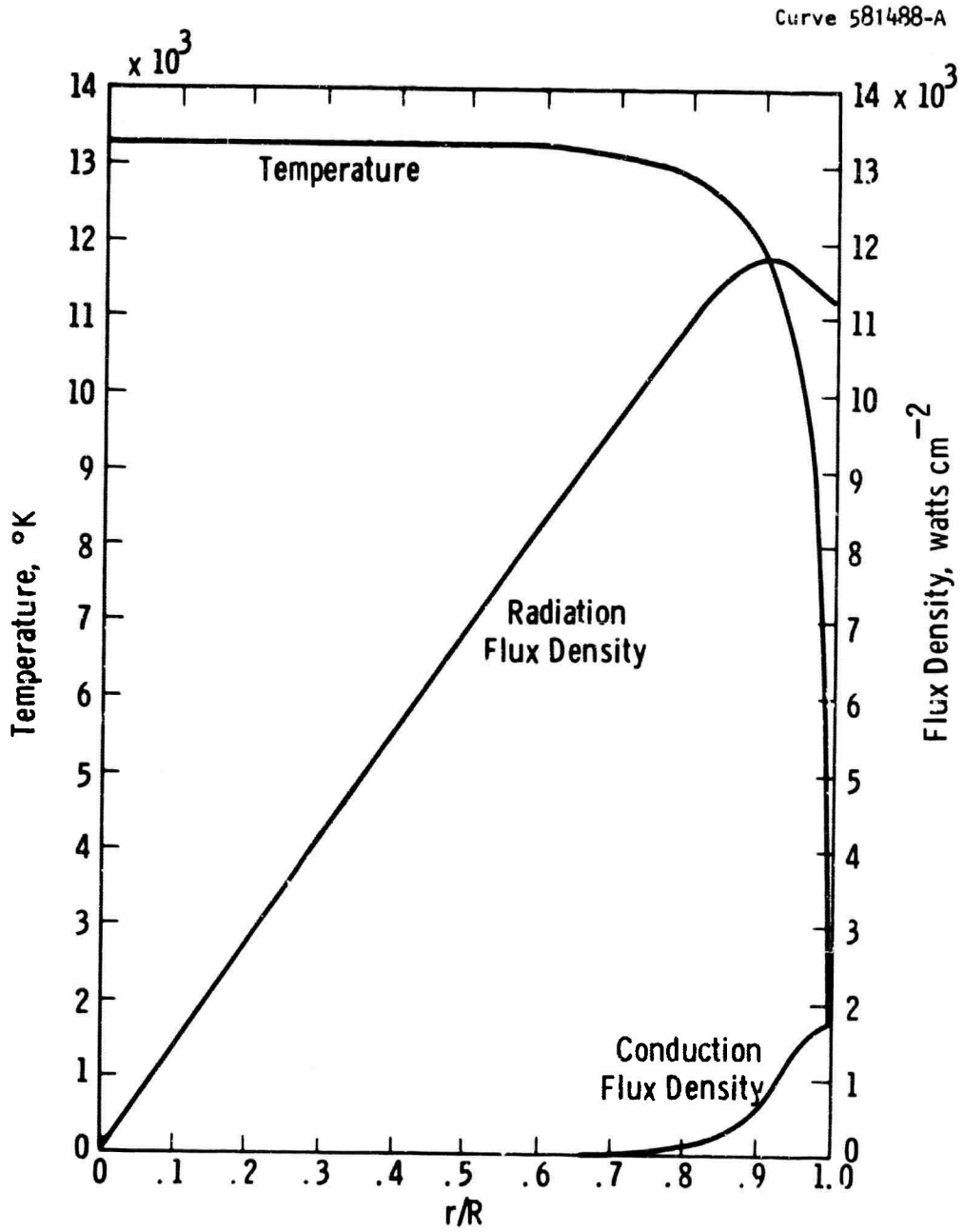

Fig. 2—Xenon arc profile

Input: p = 4 Atm, E = 29 V/cm, R = 0.411 cm, T_W = 2000°K
Output: I = 1145 Amps

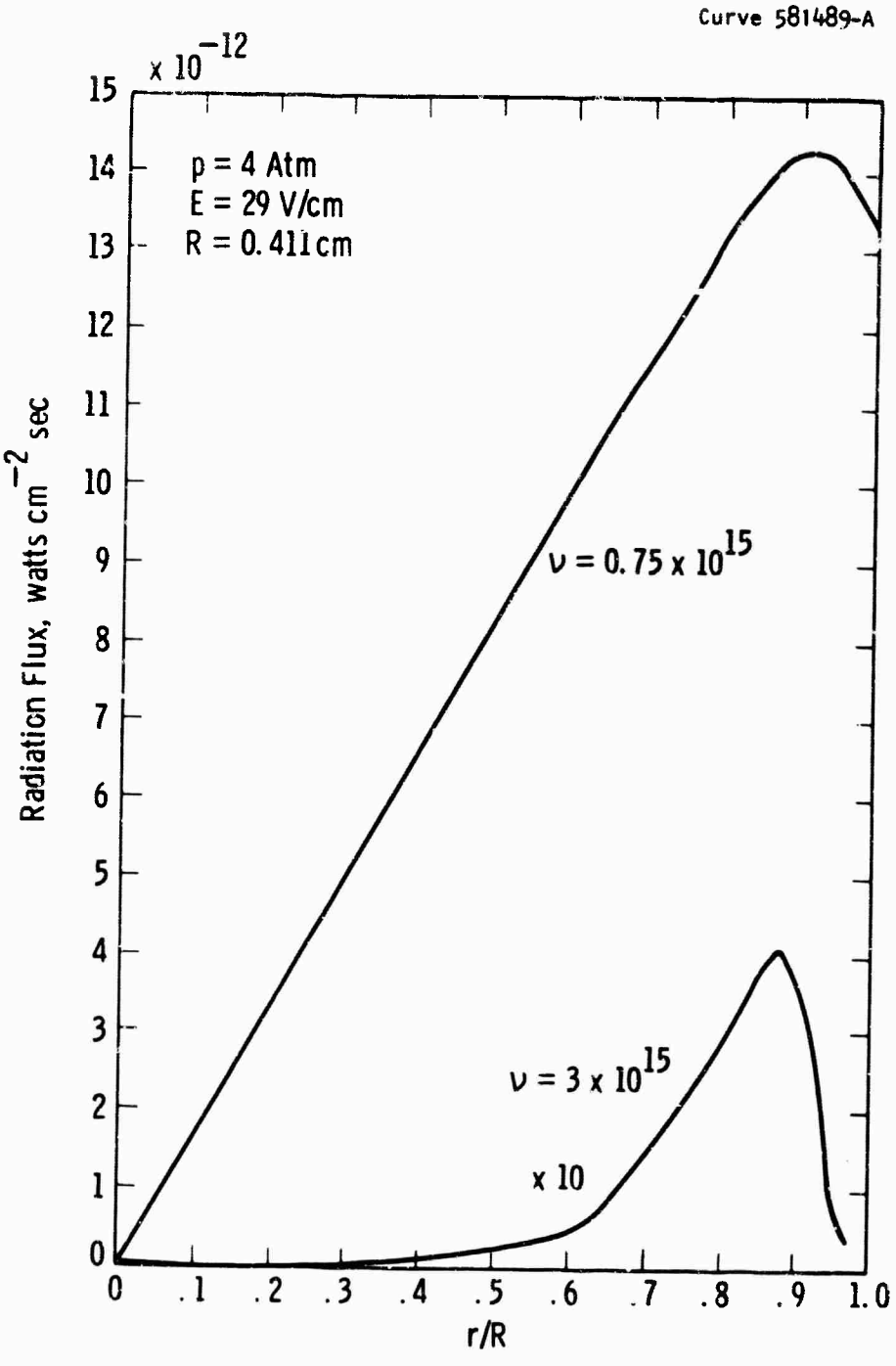

Fig. 3—Radiation flux

Curve 581490-B

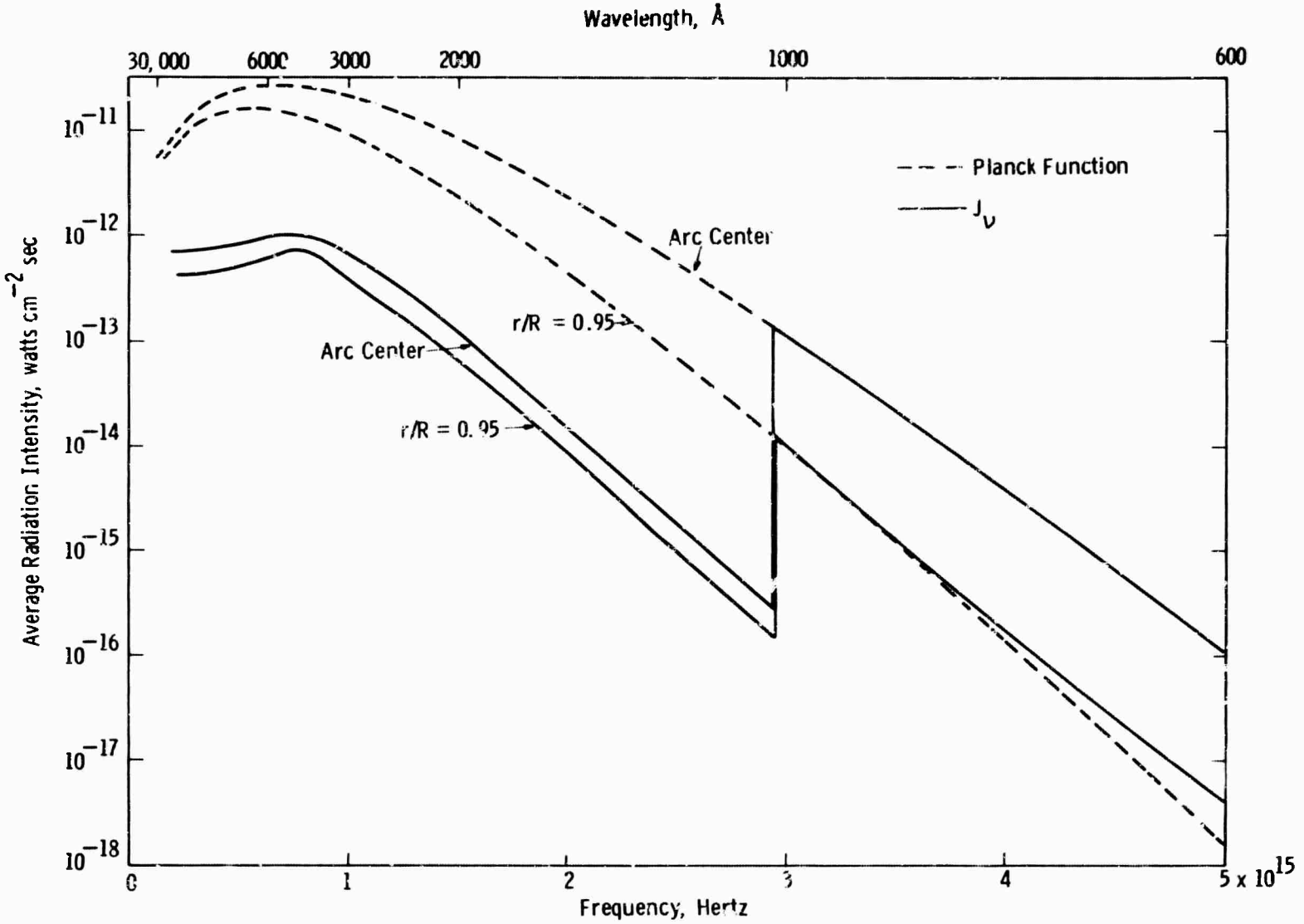

Fig. 4

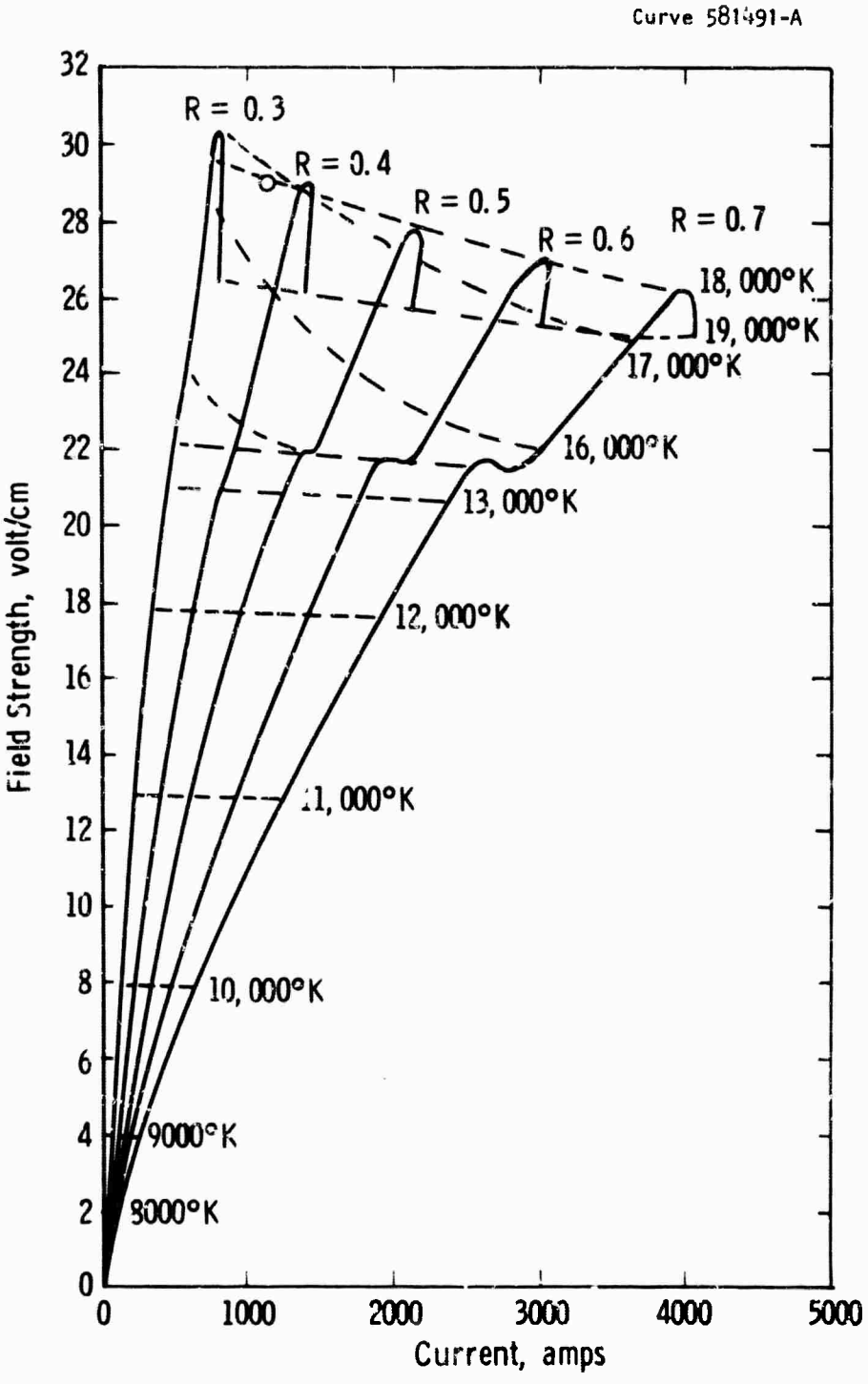

Fig. 5—Xenon, constant temp model, p = 2.5 atmospheres

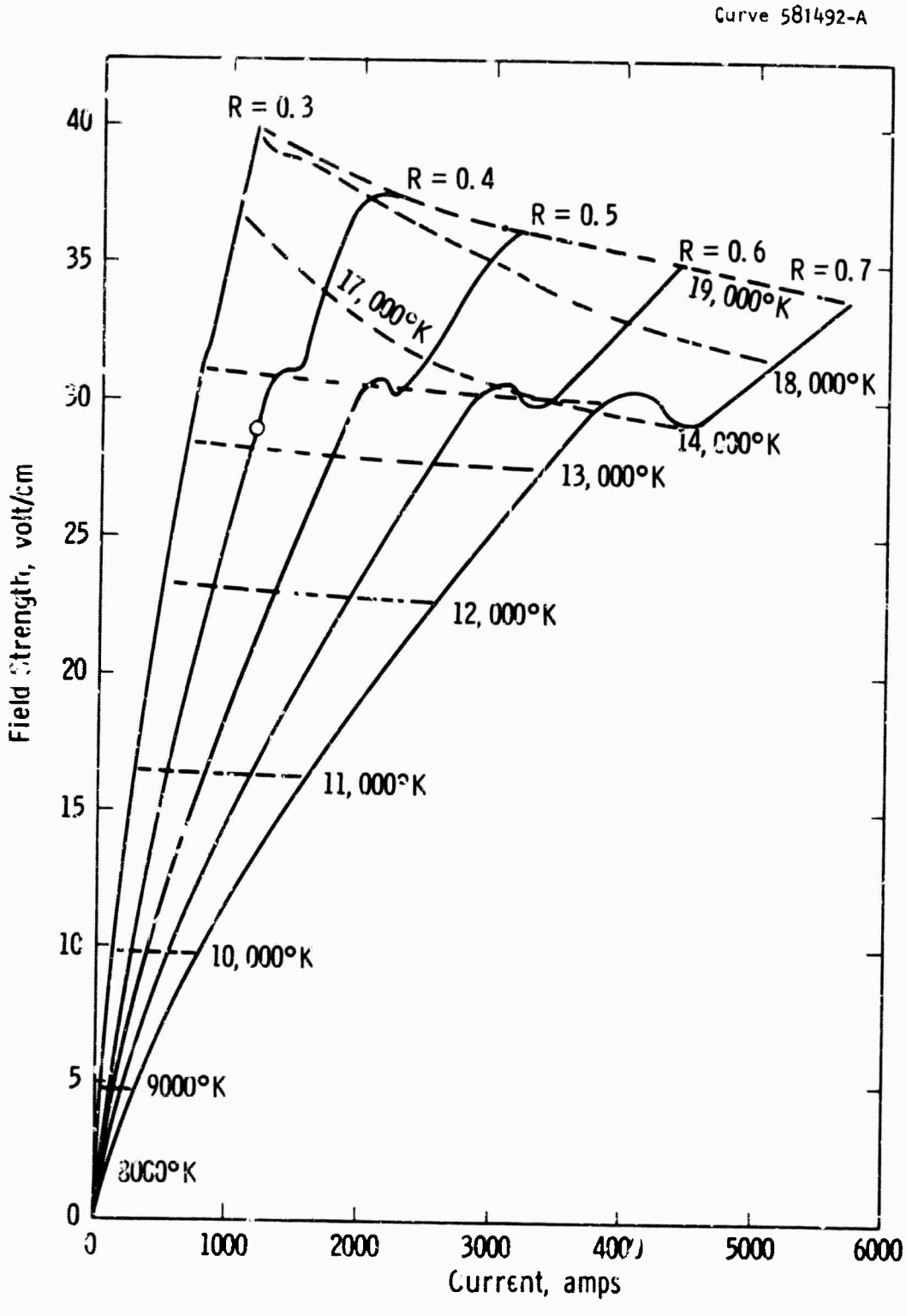

Fig. 6—Xenon, constant temp model, p = 4 atmospheres

Curve 581493-B

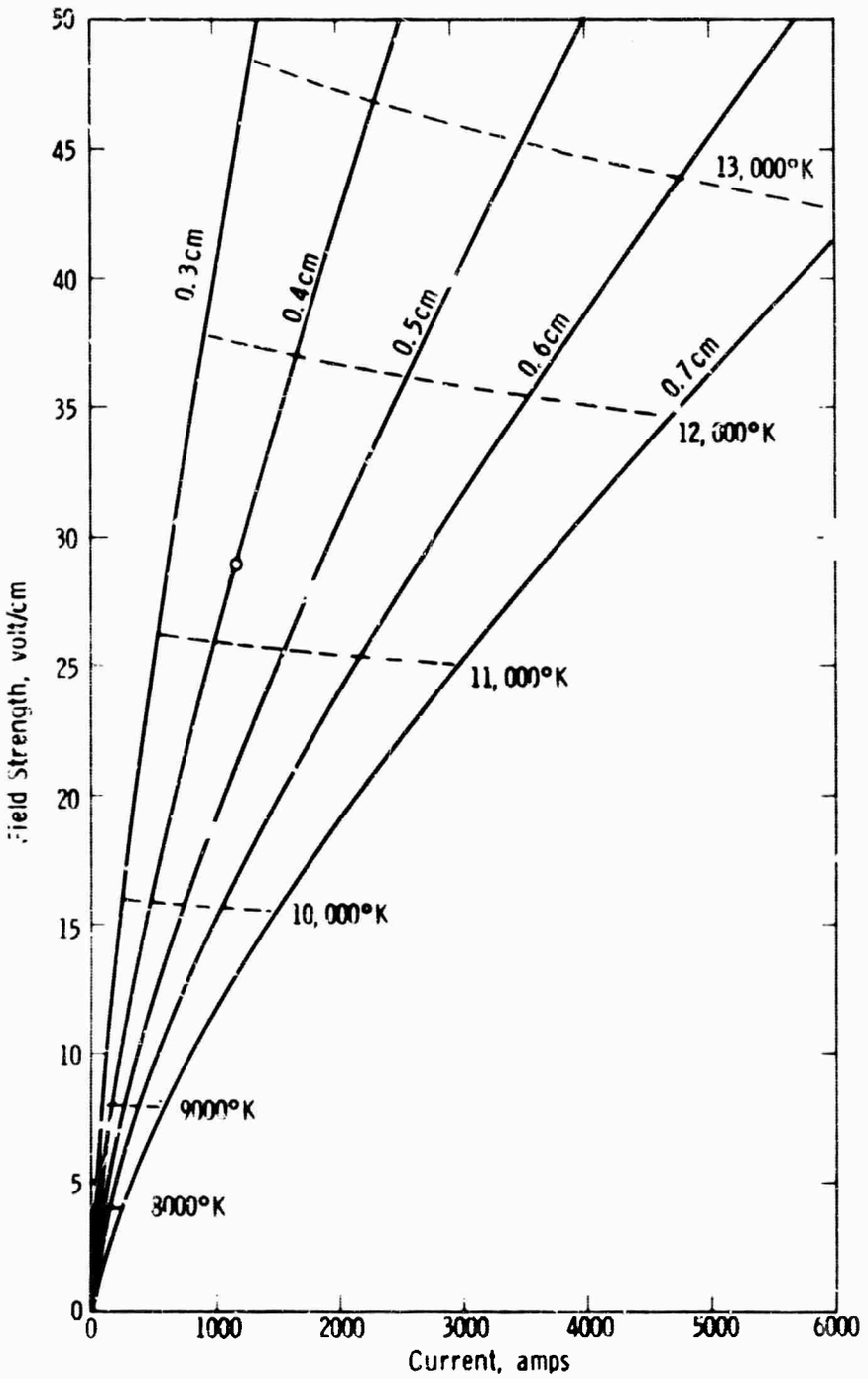

Fig. 7 – Xenon, constant temp model, p = 11 atmospheres

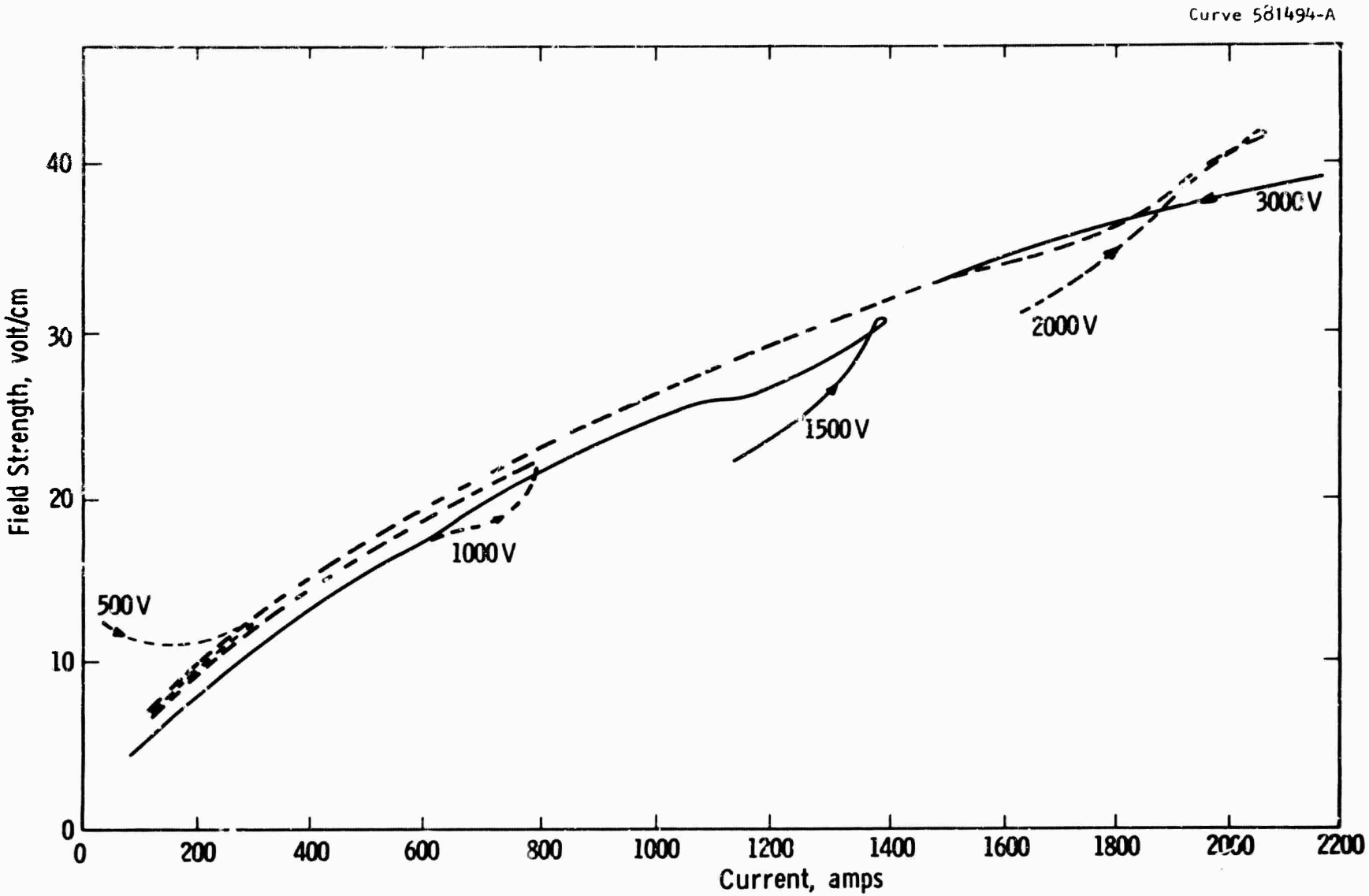

Fig. 8—Volt/current characteristic R = 0.63

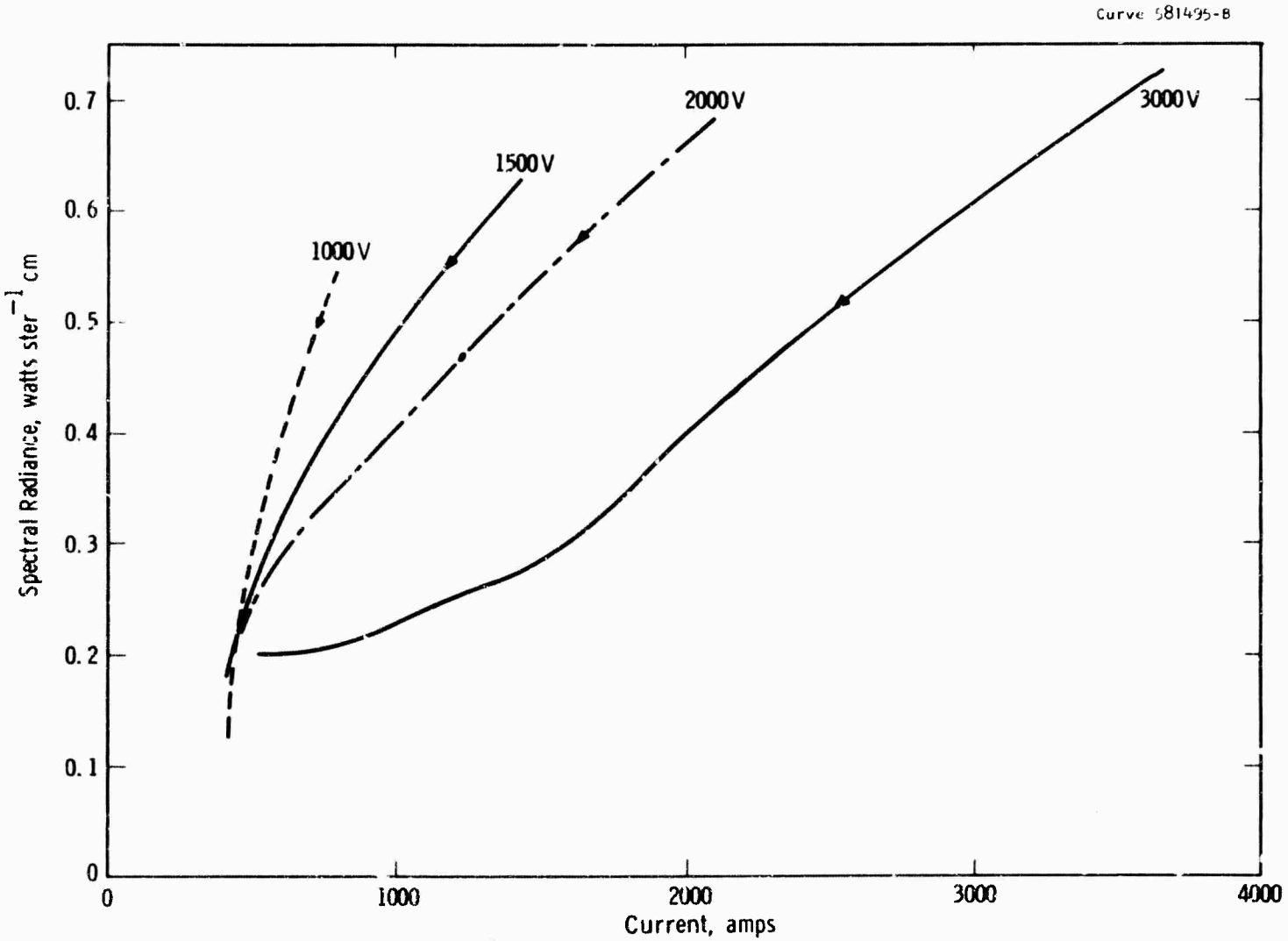

Fig. 9—Spectral radiance 8232Å

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13 ABSTRACT

This report summarizes the studies made on Contract Nonr 4647(00) towards the development of models for the highly radiative arcs used for the high energy pumping of lasers. The report also presents the experimental and theoretical studies since the last semiannual report. The experimental investigations were primarily concerned with more extensive measurements of the spectral radiance of the plasma to provide verification for the models. The theoretical work has resulted in computer methods, described in the appendices, to calculate the transport properties, the spectral absorptivities for the lines and the continuum of xenon, and the spectral radiance and temperature profiles in cylindrical arcs. Also included as an appendix is a theoretical analysis of the xenon arc using radiative transport techniques developed in other studies.

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